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**RAREFIED-CONTINUUM GAS DYNAMICS TRANSITION FOR SUMS PROJECT**

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## 1. Technical Review

Orbital vehicles at hundreds of kilometers altitude above the Earth surface are flying under a nearly vacuum condition where the mean free paths of molecular gas interactions are very large. Upon reentering the much denser atmosphere at lower altitudes, say between 160 to 60 Km, the mean free paths in the ambient atmosphere become comparable to the vehicle dimension. Only at much lower altitudes, the gaseous mean free paths become sufficiently small where continuum gas dynamics may apply. Analysis of such flow transition from free molecular to continuum conditions in connection with the reduction of data from the SUMS project is the basic theme of the contracted investigation.

Flight recordings of shuttle reentries provide the "instantaneous" acceleration data of the shuttles along their trajectories and hence the aerodynamic forces (drag and lift) they experienced. Such aerodynamic forces can be expressed in terms of the free stream dynamic head  $1/2 \rho_{\infty} u_{\infty}^2$  ( through the undisturbed gas density far away from the shuttle  $\rho_{\infty}$  and the shuttle flight velocity relative to the air  $U_{\infty}$ ), as the aerodynamic coefficients  $C_D$ ,  $C_L$  etc.. When such coefficients are assumed to be the accepted flight values in the hypersonic continuum flow regime extended into the free molecular regime smoothly, the acceleration data suggest a significant (< 50%) rise and fall of the atmospheric density around 100 Km altitude relative to the 1962 standard atmosphere. Such density stratification has been thought to be due to some gravity waves, to some unspecified anomalous energy phenomena or to some variations in atmospheric constituents etc.. There indeed might not be any atmospheric anomalies if the aerodynamic coefficients should differ from what is presumed across the transitional regime. The Shuttle Upper Atmospheric Mass

Spectrometer experiment seeks additional data to shed further light on this uncertain anomalous behavior of upper atmosphere.

Atmospheric sample is taken from the proximity of shuttle surface through a tube into a "reservoir" from which air samples are repeatedly analyzed with a mass-spectrometer. In interpreting SUMS test results to gain information about the free stream condition of the undisturbed atmosphere "far" away from the shuttle, it is necessary to relate

- (i) The state of air on the shuttle surface next to the SUMS Inlet to the undisturbed state of atmosphere far away from the shuttle - the external flow problem.
- (ii) The state of air in the "Reservoir" to that at the inlet - the internal flow problem.
- (iii) The flow rate as measured by the spectrometer to the flow rate out of the reservoir - the instrument characteristics.

The last item (iii) has been "calibrated" in the laboratory as a transfer function for the specific experimental set up.

Items (1) and (2) have to be treated through "aerodynamic" calculations or theoretical analysis based on first principles according to some suitable models. The appropriate approach to such transitional aerodynamic problems is through the solution of the Boltzmann Equation. The generalization of the Monte Carlo method of solution of the "test particle problem", like the diffusion of fast neutrons by "fixed" scattering centers, to the "many body problem" of nonlinear interaction between collective gas systems is, however, very difficult.

The popular approach of Direct Simulation Monte Carlo method (DSMC) does not solve the Boltzmann equation but proposes to simulate molecular evolution by tracking computationally the collisions among a much smaller sample, that is the Monte Carlo Particles. It relies on the Central Limit Theorem to claim that the statistical information may be approximated through repeated random sampling of the smaller ensemble. The flow field as is described by the DSMC evolves primarily through global randomization or diffusion to produce smooth or monotonic transition from the free molecular to the continuum flows. This computation intensive procedure involves many numerical parameters, which can be properly adjusted to produce desired or preconceived global results, including a "smooth" curve of drag coefficient  $C_D$  vs. Knudson number  $K_N$  that fairs smoothly from free molecular values to continuum values for such flows over a shuttle nose. In this manner, the external flow problems was considered solved, although the flow properties over the SUMS inlet do not appear consistent within themselves, a signal of large numerical errors. The DSMC method was then used to estimate the flow through the inlet tube, the internal flow problem. It diverges rapidly despite extensive numerical smoothing and wide range of choices of numerical and physical parameters including the surface accommodation coefficients. One could compute only a stagnant field in near equilibrium state in a hole but without mean flow. Under such circumstances this contract was led to develop a method for computing the internal flow fluxes through SUMS inlet tube.

The first step to make any progress is to understand what went wrong with the DSMC in the computation of the internal flow problem.

1. As the solution of an initial value problem, regardless how it is called, the CFL condition has to be satisfied to avoid numerical instability, the

DSMC simply cannot satisfy this condition for long even with excessive artificial dissipations and smoothing.

2. To make use of the Central Limit Theorem, it is necessary to have  $M K_N \ll 1$ . For the rarefied hypersonic gas dynamics problems we have, on the other hand,  $M K_N \gg 1$ . The repeated sampling while satisfying the CFL condition defies physics.

Therefore we cannot and should not attempt to make DSMC to work for the internal flow problem. The DSMC solutions are indeed dubious even for the external flow problem. We have to start from the Boltzmann equation with  $M K_N \gg 1$ , without any preconception of smooth variation from free molecular to continuum state. We have thus developed the "Beam method". For simplicity, we assume that the rare events of intermolecular collisions of the prevailing energy levels are essentially hard-ball type without exciting significant internal energy modes. The small fraction of the interacting molecules of each beam implies that the collective nature of the interacting entities, i.e. beams, will survive the highly individualized randomizing collisions under the rarefied condition. The surviving entity identified as a beam will merely reduce (or increase) its molecular population.

In principle, we should have at least three beams in our system, i.e. the two interacting beams and a product beam. For the intended applications, one of the interacting beams generated from the vehicle surface is diffusion dominated and can hardly be distinguished from the molecules after randomizing collision. Hence we simplify the model to a two beam system with intermolecular collisions as the mechanism of converting the nearly monoenergetic incident molecules into a diffusion beam. The incident beam retains its undisturbed state but with decreasing mass flux and/or mole fraction. The diffused beam will be considered

to be in quasi-equilibrium (i.e., with a distribution function approximately Maxwellian) while its effective mean flow properties evolve with the increasing mole fraction through the increased conversion of molecules from the nearly monoenergetic beam into the diffused beam.

Substituting the composite Maxwellian distribution function into the Boltzmann equation and integrating over the velocity space of each beam, we obtain the mean flow equations for each beam which resemble the Navier Stokes equations system. The departure of their distribution functions from the Maxwellians contributes to the transport coefficients according to the classical kinetic theory a la Chapman-Enskog. The mutual interaction of the two beams gives rise to external sources and sinks. The variations of the transport coefficients do not alter the basic continuum flow features. The Kyldish Institute of Applied Mathematics of the Academy of Sciences, U.S.S.R. has independently developed a similar form of continuum system which they call "Kinetic Equations" and solved computationally for some complex examples. Some literatures are being translated. The details of their developments differ from our development. We treat the highly non-equilibrium gas mixture as a mean gas with mole fraction  $\beta$  of the incident mono-energetic beam included as an additional state variable besides  $p$ ,  $\rho$  and  $T$  of the nonequilibrium gas mixture. This parameter  $\beta$  indicates the extent of progress of randomization i.e. transition to the continuum state. The time rate of change of mole fraction  $\beta$  along some average particle path or trajectory depends on the dominant collision process of randomization. It varies with different specific applications, such as the internal and the external flow problems of SUMS project.

The dominant collision process for the internal flow problem is the gas-wall surface collision. We constructed a surface interaction model based on the

presence of an equilibrium adsorbed gaseous molecular layer over the surface within the surface potential field. Then the incidence of an external molecule will lead to a "random" emission from the adsorbed layer. In this manner, incident gas molecules will be "accommodated" during gas-surface interaction, giving rise to the surface accommodation coefficients  $\sigma_t$  and  $\sigma_e$  of the tangential momentum and energy respectively with  $0 \leq \sigma_e, \sigma_t \leq 1$ . They are proportional to wall friction and heat transfer rate respectively. We do not know their values for the particular tube wall material, which values are certainly important in determining the fluxes through the tube, and should not be adjusted or selected to facilitate favorable comparison with preconceived results.

We integrated the mean flow equations across the section of the tube to reduce the Navier-Stokes system to one space dimension that governs the temporal evolution of the flow along the tube, naturally with wall friction and heat transfer included in the equations system, (and hence  $\sigma_t$  and  $\sigma_e$ ). It becomes apparent that with appropriate friction and heat transfer, the tube can become "choked" in the steady state such that quasi-steady approximation of the mass flux can be very much in error. The transient state of a "choked" tube can reduce the influx by altering the flow states upstream of the tube; thus, the "external" and the "internal" flow can be "coupled" in the analyses of SUMS Data. We may need the transfer function rather than simply the static calibration of the instrument package characteristics to those of a static reservoir. Therefore, we constructed the temporal evolution of such rarefied hypersonic flow through the tube from a selected, fixed inlet conditions for many combinations of the accommodations coefficients  $\sigma_t$  and  $\sigma_e$  into a reservoir that is presumed to be a vacuum. We only have to solve computationally the flow into a vacuum reservoir because of the near free molecular conditions inside the tube. If the reservoir



should possess some residual gas at some low pressure and temperature, this reservoir gas will create a set of fluxes out through the tube as a small flux into the external flow field without interfering with the influxes. All gaseous molecules in the tube collide with the wall surface before that might encounter any gaseous molecules away from the surface. In the transient state, the "reservoir" pressure will change with the net influx into the reservoir. The details of the formulation and the results of such computations and their discussions are given in Appendices 1 and 2. Thereby

1. We demonstrated how the internal flow problem is formulated and computationally solved.
2. We illustrated the general behavior of such solutions in the transient phase.
3. We demonstrated how the internal flow solutions vary with the accommodation coefficients  $\sigma_t$  and  $\sigma_e$ .
4. We explored and demonstrated the parametric boundary of possible "choking" of internal flow that any steady state outflow will take place only at some "reduced" influx.
5. We examined and explained how our internal flow solution can be used in the reduction of SUMS data.

A short presentation of selected results is to be published in the proceedings of the 11th International Conference of Numerical Fluid Dynamics as Lecture Series of Physics, by Springer-Verlag. A preprint of which is attached as Appendix 3. The program listing for such internal flow computations is attached in Appendix 4.

In view of the crucial role of the values of the accommodation coefficients  $\sigma_t$  and  $\sigma_e$  in determining the fluxes through the inlet tube, it is believed that

such coefficients should be determined experimentally "in situ". We have therefore proposed to have such accommodation coefficients measured directly in flight during shuttle reentry. It is a relatively simple and a highly accurate measurement as is described in Appendix 5. The measurement should be made "in Situ" because the accommodation coefficients of pure metals as measured in Laboratories are highly sensitive to the "Cleanliness" of the surface depending very much on the various degassing procedures. The adsorbed molecular layer on a solid surface is very difficult to be rid off completely; and the absorbed layer is the cumulative results of the past history of "exposure". Laboratory experiments can of course be better than "zero" information provided that the "test sample" is "treated" with suitable exposure to simulate the free flight conditions. We strongly hold the view that such coefficients should not be taken as adjustable parameters in the reduction of the data, but must be experimental determined.

The internal problem has been formulated, studied and illustrated for matching with the instrument characteristics for reducing SUMS data. We then turn our attention to the solution of the External problem with our beam method. The details of our treatment of the external flow problem from the molecular and the kinetic point of views are given in Appendix 6. It requires some model of interaction of the nearly monoenergetic incident molecules with the diffused, emitted (or reflected) molecules from the vehicle surface. We formulated such interaction at the molecular level from the view of test particle model of Monte Carlo simulation and also from the global view of scattering beams. Both give the interaction model (Appendix 6 - equation 3).

$$\rho_1 - \rho \beta = \exp \left[ - \frac{C}{K_n} \left( 1 - \frac{1}{\rho} \right) \right]$$

This interaction relation gives  $\rho = 1$  and  $\beta = 1$  at infinity for all Knudson numbers. With  $\rho$  increasing from 1 toward the surface, the density  $\rho_1$  of the undisturbed incoming beam is reduced from unity essentially exponentially with decay rate inversely proportionally to the  $K_N$  of the undisturbed stream. The scattering constant  $C$  is of order unity such that at altitudes around 120 Km with  $K_N \sim 0(1)$ , flow transition from the free molecular to the continuum state will take place. The variation of the mean flow properties of such a transitional flow are governed by equations - (3) and (4) Appendix 6. Their solution for the mean flow quantities with some detailed models of  $r_{ij}$ ,  $q_i$  and  $D$  is indeed not basically different from that of the continuum Navier-Stokes except for the boundary conditions on the vehicle surface. It is considered not appropriate in view of the uncertainties of such models and of our limited interest of the mean properties over the complex Shuttle surface, in particular over the SUMS inlet only. Therefore, we are developing an integral form of solution for the surface properties only by postulating exponential decay laws of various mean properties away from the shuttle surface. We integrate equations system (4) from surface to infinity to obtain a system of equations for the solution of the surface properties just outside the adsorbed gas layer over the Shuttle. The molecular model of interaction of incident gas with the equilibrium adsorbed molecular layer enable us to formulate the surface stresses and heat transfer rate in terms of the accommodation coefficients  $\sigma_t$  and  $\sigma_e$  of the shuttle surface.

The system of integrated equations governs the evolution of the surface flow properties along the shuttle surface in two space dimensions. The mean tangential gas velocity increases from zero at the stagnation point near the axis to the highly supersonic condition on the shuttle surface far away from the axis. A subsonic region must exist around the stagnation point, bounded by a closed

sonic curve on the surface where some special condition must hold if the solution is to pass through smoothly. The location of this sonic point on the surface relative to the SUMS Inlet can have far reaching consequences on the inflow through the tube to the Mass-Spectro-meter, especially if SUMS inlet is to be swept over by this sonic curve during shuttle's descending trajectory.

## 2. Current Status

The solution internal flow problem has been fully developed. Given the inflow into the inlet tube and the accommodation coefficients  $\sigma_t$  and  $\sigma_e$  of the tube wall, we can calculate the evolution of the flow through the inlet tube into a vacuum reservoir. The program of such a computation is enclosed as Appendix 4. If the reservoir should have a residual equilibrium gas, there will be an outflow of gas molecules from the reservoir through the inlet tube into the external flow field. In the absence of gaseous interaction, the inflow and outflows are totally independent and can be calculated separately. The difference of the influx into and the outflux from the reservoir through the inlet tube is the net influx into the reservoir to be matched with the instrument characteristics. The computed evolution of the inflow is of very fine time scale to permit matching with any transient characteristics of the instrument package if available.

If the inflow is unchoked, the inflow will quickly ( $\sim 10^{-3}$  sec.) reach a steady state for matching with the quasi-steady instrument characteristics. If the inflow is choked the reflected waves from the choked inlet flow will alter the flow states external to the SUMS inlet to reduce the inflow. If the external flow over the SUMS Inlet is stable, a steady state with reduced influx will eventually be reached. Whether the matching to the instrument characteristics

may be considered quasi-steady or transient depends on the characteristic response time of the instrument package. If the external flow over SUMS inlet should be "unstable", the external and the internal flows would be intimately coupled and the transient matching would be imperative.

The system of flow equations integrated over the flow (or flight) direction from the shuttle surface to infinity is still much too complicated for demonstrating and studying the external flow solution. Therefore, we introduce further the tangent cone approximation with the conical body tangent to the shuttle surface along the meridian section containing the SUMS Inlet. The conical axis is the flight direction. This external flow problem has been formulated and programmed for numerical solution of the surface mean properties, along the meridian arc. Preliminary results confirmed the sensitivity of the numerical solution to the initial data and the likely presence of a strong "sonic" singularity (Appendix 6). The location of this sonic singularity clearly depends on the Knudson number and the accommodation coefficients. The SUMS Inlet located at  $\sim 32^\circ$  off the geometric axis of the Shuttle, will likely be traversed over by this transonic singularity as the  $K_N$  decreases from large values  $K_N \gg 1$  for free molecular to small values  $K_N \ll 1$  for continuum flow. When the sonic point sweeps over SUMS Inlet, the flux into the inlet tube will likely undergo some significant change. We have not yet had the opportunity to demonstrate all these through numerical computations. Some Soviet literature (being translated) on the computational solution of their kinetic equations in multi - dimensions appear to suggest the inevitable presence a local subsonic region closed by a sonic boundary over the blunt nose. Where this transonic line will strike the surface is much affected by the surface characteristics, its geometry, its heat transfer condition, and the accommodation coefficients. We are quite certain that some

experimental determination of the accommodation coefficients of the shuttle exterior surface is essential to the solution of the external flow problem (just as those for the inlet tube surface to the solutions of the internal flow problem).

Our position with respect to the surface accommodation coefficients in the treatment of the external flow problem is much different from that of the popular DSMC computations. The DSMC computations presents a straight-forward and hence attractive although tedious approach of the external flow-problem through simulated gas-gas collisions, and supposes that the surface accommodation coefficients of the gas-surface interaction can be adjusted so as to reproduce pre-conceived results or available experimental data. With the gas-surface interaction an essential part of our model, we consider the surface accommodation coefficients as surface properties which must not be manipulated to fit results.

The presence of an adsorbed molecular layer over any solid surface is central to the surface-gas interaction model adopted in our analysis with the accommodation coefficients proportional to wall friction and heat transfer. This adsorbed layer of microscopic dimension provides the physical basis of the "Nonslip" condition on a solid surface in a continuum gas, and of the "Slip" condition when the gas becomes rarefied and departs from the continuum condition. Under the highly rarefied conditions the accommodation coefficients replace the viscosity and the heat conductivity coefficients of gas continuum and our model of equilibrium adsorbed layer for highly rarefied gas replaces the gradient diffusion type model of friction and heat transfer in the continuum. The presence of such an absorbed molecular layer with its thickness much less than the gaseous mean free path is most evident in catalytic surface reaction in

rarefied gas, such as the reaction of oxygen with hydrogen adsorbed on platinum surface (to be published "Progress in Energy and Combustion Sciences" - An International Review Journal - Appendix 7) in space propulsion systems. The change over of the second order kinetics of the binary gaseous reactions of oxygen and hydrogen to the first order kinetics of catalytic surface reaction suggests the presence of the high density molecular hydrogen layer adsorbed on Pt surface, independent of the gas density. Surface adsorption is a highly selective process but is surely present between any gas-surface pairs. (The difficulty of cleaning a solid surface of its prior gaseous exposure testifies to the tenacity of such an adsorbed layer). The accommodation coefficients are the results of molecular interaction within the adsorbed layer and could in principle, be estimated from detailed atomic structural data. There is little reason to believe that such accommodation coefficients (or the viscosity and the heat transfer coefficients) in rarefied (or the continuum) gas dynamics could be treated as adjustable numerical constants as is in DSMC. This is why we have proposed the experiment for their determination as described in Appendix 5.

## Conclusions and Suggestions for Future Investigation

The primary objective of the original contracted investigation for developing a method of computational solution of the internal flow problem to facilitate the analysis of SUMS data has been fulfilled.

The details of matching this internal solution to (1) the instrumental package and (2) to the external flow solution over SUMS inlet are awaiting the appropriate characteristics of the instrument package and the flow states over SUMS Inlet.

Our attempt to develop a method for analyzing the external flow problem as an alternative to DSMC is partially completed but untested.

Our investigation brings out the essential role of surface accommodation coefficients for both the shuttle external surface material and the inlet tube material in air in the reduction of SUMS data. We suggest therefore the following investigations in preparation for the eventual analysis of SUMS data:

1. Continue the development of the external flow solution methods by carrying out the numerical example in progress and generalize, if necessary to Shuttle Geometry for the direct determination of the flow properties over the SUMS Inlet.
2. Carry out the in situ determination of the accommodation coefficients of the appropriate materials as proposed in Appendix 5 or other laboratory determinations.
3. Establish the matching procedures for joining:
  - (i) the flow states at the inlet tube exit and the instrument package characteristics;
  - (ii) the flow states over the SUMS Inlet as given by the external flow solution and the inflow into SUMS Inlet tube for both the choked and the unchoked internal



flow configurations.

## Appendix I.

### SUMS Internal Flow Formation

The internal flow problem of SUMS project refer to the flow through a  $\sim 0.2$  cm. diameter, straight vylcor-tube of about 10 cm. long connecting the tube inlet from the shuttle tile surface to a downstream "reservoir". Gas samples are drawn from the reservoir for analysis and direct measurement in the mass-spectrograph. The analysis of the rarefied gas flow through the tube is to relate the flow state at the tube exit into the reservoir to the states at the SUMS inlet on the Shuttle surface along its descending trajectory below say 200 Km altitudes. At the lower altitudes, when the atmospheric flow along the shuttle surface is generally in the continuum range with the local mean free path comparable to or somewhat smaller than the shuttle exterior dimensions, the gaseous mean free path is still much larger than the tube diameter. Accordingly, intermolecular gaseous collisions are rare events in comparison with the gas-wall collisions brought about by the the random components of molecular gas motion in the plane transverse essentially free molecular while being randomized through the much more frequent gas-wall interactions. Therefore the wall surface conditions and the "law of interaction of incident gas molecules with the solid wall" are more important.

We know little about the surface condition except that it is "contaminated" and covered with a molecular layer of adsorbed gas molecules due to previous exposure. These molecules are held together by the surface potential, absorbed and fully accommodated to the surface temperature. An incident molecule will collide with the adsorbed molecules, leading to the emission on the average an adsorbed molecule from the equilibrium layer that is a unit yield. Since the incident molecules carry on the average a significantly larger amount of momentum and energy, it is likely that the incident molecules will have lost to the adsorbed layer on the average some fraction of their excess momentum and energy. We call those fractions  $\sigma_t$  and  $\sigma_e$  the accommodation coefficients for the tangential momentum and the total energy respectively. They stand as the wall

friction and wall heat loss parameters in the rarefied regime. The component of momentum normal to the surface is presumably annihilated and the emission of adsorbed molecules from the solid surface is "thermal" or diffused at the surface temperature. The temperature of the tube wall is supposed to be known. The physical properties of the tube wall of present concern are thus only the two accommodation coefficients  $\sigma_t$  and  $\sigma_e$  for the tangential momentum and the total energy. Clearly both  $\sigma_e$  and  $\sigma_t$  should not be taken as the experimental values for "clean solid surface" but those with adsorbed molecular gas layer under the prevailing circumstances. We do not know how to specify this "Dirty" Surface condition other than the relevant values of  $\sigma_t$  and  $\sigma_e$  themselves.

The one dimensional flow consists of two interacting beams. Each of the two beams is assumed to be in quasi-equilibrium and governed by the Navier-Stokes type equations. The gas-wall collisions lead to various sources in these equations. The thermodynamic and the kinematic states  $(p_1, e_1, u_1)$  of the uncollided beam (subscript 1) remain unchanged from the tube entrance downstream while its population or density  $\rho_1$  decreases along the tube because of the randomizing collisions with the tube wall under their thermal motion. Under the assumption of unit yield upon wall collisions, the decrease in  $\rho_1$  is accompanied by a corresponding increase in  $\rho_2$  as the molecule(s) in the uncollided beam 1 is converted into a new molecule(s) in the diffused beam 2. This conversion of beam 1 molecules into beam 2 and the interaction of the beam 2 molecules themselves with the wall lead to changes in the thermodynamic and the kinematic state of beam 2.

It is convenient to consider the mixture of the two quasi-equilibrium beams as a "Pseudo-equilibrium" gas mixture with global density

$$\rho = \rho_1 + \rho_2 \quad (1)$$

of the same kind of molecules in different quasi-equilibrium states 1 and 2.

We assign the mole fraction  $\beta$

$$\beta = \rho_1 / \rho \quad (1a)$$

of the uncollided beam 1. So that the mole fraction of the diffused beam 2

$$\text{becomes} \quad 1 - \beta = \rho_2 / \rho \quad (1b)$$

Likewise, we can define the pressure of the gas mixture as

$$p = p_1 + p_2 \quad (2)$$

$$\text{with } p_1 = \beta p \text{ and } p_2 = (1 - \beta)p \quad (2a,b)$$

These relations are compatible with the conventional notion of partial pressure and partial density. Both the mean and the individual beam of gas can follow the equation of state of an ideal gas with the same gas constant R

$$\begin{aligned} p &= p_1 + p_2 = \rho_1 RT_1 + \rho_2 RT_2 \\ &= \rho R[\beta T_1 + (1 - \beta)T_2] = \rho RT. \end{aligned}$$

if the mean gas temperature T is defined as

$$T = \beta T_1 + (1 - \beta)T_2 \quad (3)$$

Note that the temperature of each gas should not be interpreted as partial temperatures. If both beams of gas molecules are taken to be identical and possess the same average specific heat at constant volume

$$C_v = R/(\gamma - 1) \text{ such that}$$

$$e_1 = C_v T_1 \text{ and } e_2 = C_v T_2 \quad (3a,b)$$

we have

$$\beta e_1 + (1 - \beta)e_2 = C_v[\beta T_1 + (1 - \beta)T_2] = C_v T$$

$$\text{or} \quad e = C_v T = \beta e_1 + (1 - \beta)e_2 \quad (3c)$$

The mean gas will have the same  $C_v$  as the individual gas components. Thus all the thermodynamic properties of the mean gas are consistently defined in terms

of the mole fraction  $\beta$ . Despite the non-equilibrium structure of the "gas mixture", it can be treated as a "mean gas."

The mean velocity of the "mean gas" will be defined in terms of momentum as

$$u = (\rho_1 u_1 + \rho_2 u_2) / \rho \quad (4)$$

$$\text{i.e.} \quad u = \beta u_1 + (1-\beta)u_2 \quad (4a)$$

Upon integrating over the tube section, the 1D continuity equation for each beam results. The sum of the two gives the continuity equation for the mean gas

$$\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x} \rho v = 0 \quad (5)$$

where unit yield of incident molecules on wall makes the source term vanish. Similarly we obtain the 1-D momentum and the energy equations of the mean gas:

$$\frac{\partial}{\partial t} \rho u + \frac{\partial}{\partial x} (\rho u^2 + p) = -4\tau_w \quad (6)$$

$$\frac{\partial}{\partial t} \rho e + \frac{\partial}{\partial x} (\rho e + p) u = -4 \dot{q}_w \quad (7)$$

in which the wall stress term  $\tau_w$  and heat transfer term  $\dot{q}_w$  are to be evaluated from the detailed model of wall interaction. The momentum flux term  $\frac{\partial}{\partial x} \rho u^2$  in (6) contains the mutual interaction term  $\frac{\partial}{\partial x} [\beta(1-\beta)\rho(u_1-u_2)^2]$  in addition to  $\frac{\partial}{\partial x} (\rho_1 u_1^2)$  and  $\frac{\partial}{\partial x} (\rho_2 u_2^2)$ . Similar mutual interaction terms of energy flux are present in the energy equation (7). Such terms vanish as  $\beta \rightarrow 0$  and  $\beta \rightarrow 1$  and are presumably small at least when compared with the wall contributions. The inclusion or omission of such mutual interaction terms may have distorted the effective values of

the accommodation coefficients  $\sigma_t$  and  $\sigma_e$  which we know so little about. We choose to ignore such differences and leave equations (5) - (7) in the conventional form of gas dynamics equations to facilitate physical understanding. Both  $\tau_w$  and  $\dot{q}_w$  depend on the details of wall interaction of incident molecules from the two beams. The wall interaction is the result of transverse migration under the thermal velocities  $c_1$  and  $c_2$  of the respective beam of molecules. The transversal migration of beam 1 molecules to collide with tube wall leads to their disappearance and conversion into beam 2 molecules.

Thus,

$$\frac{d}{dt} (\rho\beta) = \frac{\partial}{\partial t} (\rho\beta) + \frac{\partial}{\partial x} (u\rho\beta) = -\rho\beta c_1 \quad (8)$$

In terms of the accommodation coefficients  $\sigma_t$  and  $\sigma_e$  introduced earlier, we have the wall friction and the wall heat transfer parameters:

$$4\tau_w = \rho\sigma_t [\beta c_1 u_1 + (1-\beta) c_2 u_2] \quad (9)$$

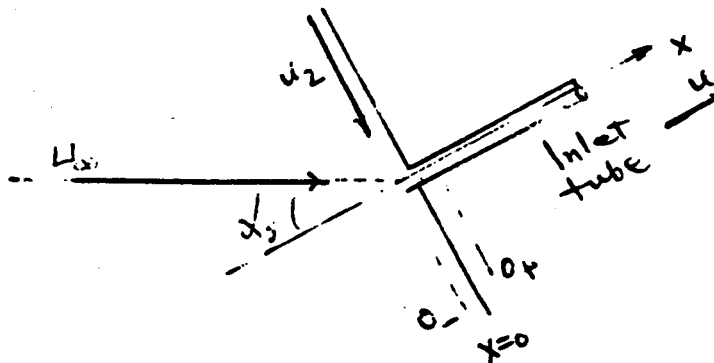
$$4\dot{q}_w = \rho\sigma_e \left[ \beta c_1 \left\{ (e_1 + \frac{u_1^2}{2}) - (e_w + \frac{(1-\sigma_t)^2 u_1^2}{2}) \right\} + (1-\beta) c_2 \left\{ (e_2 + \frac{u_2^2}{2}) - (e_w + \frac{(1-\sigma_t)^2 u_2^2}{2}) \right\} \right] \quad (10)$$

where the velocity, the density and the internal energy (or temperature at constant specific heat) are nondimensional expressed in terms of their corresponding values of the undisturbed free stream at infinity (far away from shuttle). The pressure is nondimensional in terms of the free stream dynamic head  $\rho_\infty U_\infty^2$ . The tube diameter is taken as unit length. The reference time is taken as the transit time for the freestream  $U_\infty$  to traverse the tube diameter, an extremely small quantity.

Equations (5), (6), (7) and (8) are the set of partial differential equations governing the evolutions of  $\rho$ ,  $e$ ,  $u$  and  $\beta$  as functions of  $x$  and  $t$ .

The wall friction and heat transfer  $4\tau_w$  and  $4\dot{q}_w$  are given explicitly as the subsidiary relations (9) and (10). It stands as a pure initial value problem, i.e. given the initial data of  $\rho$ ,  $e$ ,  $u$  and  $\beta$  immediately behind the tube entrance at  $x = 0_+$ , the flow states throughout the tube at later times are entirely determined regardless of the tube exit conditions within the transient framework. It will be the ultimate solution if the reservoir is a vacuum. The implication of some nonzero gas pressure in the reservoir will be discussed later separately.

The state of the gas flow at  $x = 0_+$  is distinguished from that immediately outside the tube entrance  $x = 0_-$ , where the gas flow is not "one dimensional". It consists of two beams: a nearly monoenergetic stream of velocity  $U_\infty$  at an angle  $\alpha_s$  with the tube axis and a diffused stream with a mean velocity  $u_2$  tangent to the shuttle surface at the tube entrance  $x = 0_-$  normal to the tube axis.



The mono-energetic beam 1 provides at  $x = 0_+$  a high energy beam with a mean velocity  $u_{10} = U_\infty \cos \alpha_s$  along the tube axis at a temperature

$$T_{10} = T_\infty + \frac{\gamma - 1}{\gamma} \frac{U_\infty^2 \sin^2 \alpha_s}{2R}.$$

The kinetic energy associated with the directed motion  $U_\infty \sin \alpha_s$  normal to the tube wall is converted into heat through collision with the tube wall in the proximity of the SUMS inlet  $x = 0_+$ . The mole fraction will be taken as

remaining unchanged, i.e.  $\beta_{0-} = \beta_{0+} = \beta_0$ . The flow of the diffused beam 2 into the tube is due to the half Maxwellian thermal velocity incident onto the Shuttle surface near the SUMS inlet. The mean velocity of the half Maxwellian influx along the tube axis  $U_{2n} = c_{20}$  (normal to shuttle surface locally) is taken to be the inlet mean velocity of beam 2. The kinetic energy associated with the tangential component of the mean motion  $u_{2t}$  tangent to the shuttle surface is converted into heat upon entering the tube (through collisions with tube wall). Thus

$$T_{20+} = T_{20-} = T_{2t-} + \frac{\gamma-1}{\gamma} \frac{U_{2t}^2}{2R}$$

with the total energy of beam 2 molecules unchanged. The conversion of the quasi-equilibrium flow in 3D just outside SUMS inlet ( $x = 0_-$ ) to a 1-D quasi-equilibrium flow just inside SUMS inlet ( $x = 0_+$ ) is very complex and takes place in a very short span of space-time. The procedure described above is constructed to conserve the appropriate global quantities which are deemed important in determining the fluxes through the inlet tube. The inlet flow conditions are presumed to be constant (steady) during each period of sampling for analysis by the massspectrograph. The outer solutions of the flow field over the shuttle at a given altitude is supposed to provide the flow conditions at the SUMS Inlet with the inlet opening closed, i.e. the state of the gas just outside the adsorbed molecular layer on the tile covering the inlet. The outer solution permits the evaluation, at the inlet  $x = 0_+$  of the nonequilibrium parameter  $\beta$ , and the mean flow properties  $u$ ,  $T$  and  $\rho$ .

For the solution of the initial value problem, we need further the initial data at  $t = 0$  throughout the entire tube length  $55 > x > 0_+$ . We assume that all quantities take the inflow values at the inlet  $x = 0_+$  at time  $t = 0$ . We



also presume that the "reservoir" pressure just beyond the exit of the inlet tube is sufficiently small to accept whatever mass flux that may come out of the tube exit. With the wall temperature  $T_w$  and the wall accommodation coefficients  $\sigma_e$  and  $\sigma_t$  given the evolution of the dynamic and flow state variables,  $\beta$ ,  $\rho$ ,  $u$ ,  $e$  (or  $C_v T$ ) throughout the tube is mathematically defined for all the later times, so long as all the parameters in the initial boundary data are held constant. Some quasi-steady flow state may be reached if the reservoir is maintained at some steady condition. The uniform initial flow at  $t = 0$  in our computations may look artificial. For different sets of initial data at  $t = 0$ , the ensuing solutions at early times will surely be different. It is yet to be demonstrated that they will soon become essentially the same at later times when the precise course of evolution is determined by the steady flow condition.

We are presently interested in studying the analytic behavior of the solution and the relative importance of the different parameters in determining the internal flow solution. With such information, we can better handle the actual reduction of SUMS data by focusing our attention on such important parameters. We first note that the system of equations (5) - (10) is "linear" in  $\rho$  so that all the other properties are independent of the initial magnitude of the global density  $\rho_0$  of the gas entering the inlet tube. Accordingly, we can arbitrarily take that global density to be unity in our parametric study. The relevant parameters from the outer solution are thus  $\beta$ ,  $u$  and  $T$  only. The most important parameter is likely  $\beta$ , designating the extent of non-equilibrium, i.e. the fraction  $\beta$  of the nearly monoenergetic beam of gas not yet collided with any other gaseous molecules. These molecules in beam 1 will enter directly into the inlet tube with a significant velocity component normal to the shuttle surface. Any inflow from

the diffused beam into the inlet tube is due to the thermal motion of the diffused molecules. The relevant parameters from the wall are the wall accommodation coefficients  $\sigma_t$  and  $\sigma_e$ , which represent respectively the wall friction and the wall heat transfer parameter along the tube. With sufficiently large friction and small heat loss of a long tube, the mass outflux at the tube exit can be much less than the mass influx at the inlet. The excess mass influx must accumulate in the tube somewhere, with rising pressure tending to stop or even reverse the flow. These "pressure waves" will soon pass upstream out of the inlet to alter the flow states just outside SUMS Inlet. Such an event is the transient associated with "Chocking" of the quasi-steady one-dimensional flow. We shall therefore refer to such transient events of developing local negative mass flux anywhere in the tube "Choking."

For a given set of inflow conditions  $\beta$ ,  $u$ ,  $T$  and the wall accommodation coefficient  $\sigma_t$  and  $\sigma_e$  for the given tube Wall temperature, the internal flow and its outflux into the reservoir can be determined as the solution of the initial boundary value problem described above. If the parameters are such that the inlet tube is choked, the external flow and the tube inlet conditions will be modified by the upstream propagating pressure waves with consequent changes of mass influx into the tube and mass outflux into the reservoir. It is thus important to find out if choking would take place, i.e. if the parameteric boundary of choking should overlap the physical range of interest. When the inlet tube is choked, the inner and the outer flow field are coupled such that the determination of the out flux from the inlet tube into the reservoir will involve iterative if not simultaneous solution of the external and the internal flow problems.

## Appendix 2.

### Unchoked Internal Flow Solutions (parametric study)

We choose the inlet flow conditions provided by Bienkowski's Monte Carlo solution at shuttle altitude 115 Km for the parametric study of the internal flow solution according to our two beam model. The immediate objectives of the study are:

1. Demonstrate how such internal solution may be obtained computationally and how extensive will be the requirement of computational resources.
2. Illustrate the general behavior of the solution in the transient phase.
3. Explore the dependence of the internal solution and the outfluxes from the inlet tube into the reservoir on the wall parameters  $\sigma_t$  and  $\sigma_e$ .
4. Explore the parametric boundary (in terms of  $\sigma_t$  and  $\sigma_e$ ) of possible "choking" of the internal flow.
5. Examine how the outfluxes from the internal solution may be determined by a steady reservoir condition, or the transfer function of quasi-steady reservoir for the reduction of SUMS Data.

The Monte Carlo solution of external flow gives the number density (molecular)  $\rho$  and the molecular distribution functions  $f_g(u_t)$  and  $f_g(u_n)$  of the gas over SUMS Inlet, assumed to be "closed" (i.e. no in or out flux of gas molecules). We assume that the molecules with positive normal velocity component ( $u_n > 0$ ) will enter the SUMS Inlet. At this altitude, we have the shuttle speed  $U_\infty = 7486$  m/sec at an angle  $\alpha_\infty = 32^\circ$  from the geometric axis of the shuttle. The shuttle tile temperature is taken as  $T_g = 510^\circ\text{K}$  with the undisturbed atmosphere at  $T_\infty = 304^\circ\text{K}$  and number density  $N_\infty = 9.83 \times 10^{17}$  in

the external flow solution. The distribution functions  $f_s(u_t)$  and  $f_s(u_n)$  from the DSMC computation display second peaks at velocity ( $u_t$ ,  $u_n$ , 0) that can be easily identified as the undisturbed incident free stream molecules, i.e. beam 1, nearly monoenergetic, undisturbed free stream molecules. These second peaks are, however, significantly broader than what the free stream temperature  $T_\infty = 304^\circ$  would indicate. While physically disturbing, we ignored them as uncertainties in the DSMC computation for this particular example that may be alleviated in future computations. We then evaluated the area of the second peak over the basic Maxwellian distribution and expressed as a fraction of the total area under the  $f_s(u_t)$ . This ratio is the mole fraction  $\beta_{O-}$  just outside the SUMS Inlet. Likewise we evaluated this  $\beta_{O-}$  from  $f_s(u_n)$ . They turn out to be 0.37 and 0.22 respectively although they should be the same. This internal inconsistency of the DSMC results is of more serious concern than the accumulation of random computation errors. We certainly hope that such inconsistency can be eliminated in the DSMC external solutions in the reduction of SUMS data. For the present purpose of parametric studies, we take  $\beta = 0.37$  and determine the mean velocities of the Maxwellian fit of the diffused stream  $U_{t2}$ ,  $U_{n2}$  and the mean temperature  $T_2$  in some consistent manner. It is fortunate that we do not have to compromise further in choosing the mean gas density  $\rho$  for the present parametric study. When converted into inflow data inside the inlet tube at  $x = 0_+$ , as described in the previous sections, the mean velocity is  $U_{O+} = 0.48$ . With the density taken as unity, the mean temperature and pressure are equal  $T_{O+} = P_{O+} = 11$ . The mole fraction  $\beta_{O+} = 0.37$ .

The quasi-steady flow of a subsonic stream through a tube of constant sectional area with friction but no heat transfer tends to become sonic and choked while a supersonic stream will go through a "Shock transition" within a

few mean free paths, (i.e. a few tube diameter) to become subsonic. If there were no wall friction and heat loss with  $\sigma_t = \sigma_e = 0$ . (i.e. perfectly elastic collision or specular reflection) from here on the downstream flow would remain unchanged, subsonic all through the tubes. If the wall friction should be very large ( $\sigma_t \approx 1$ ), the incident molecules should lose all or most of its tangential momentum upon colliding with the wall layer; the downstream mean flow velocity would be almost zero and surely remain subsonic and unchoked. Away from such extreme situations, quasi-steady 1-D flow in a tube of constant area suggests that friction tends to increase the average flow Mach number while wall cooling tends to reduce it. The temperature of the tube wall was specified to decrease rapidly from the tile temperature  $\sim 510^\circ\text{K}$  to the temperature of the interior supporting structure  $\sim 300^\circ\text{K}$ . Both are significantly less than the stagnation temperature of the gas in the tube. If cooling is not strong enough to keep the downstream from becoming sonic before reaching the tube exit, the downstream flow in the tube could be choked to produce unsteady transients and the inlet data may have to be altered. There is no good reason why quasi steady-state would be reached in SUMS inlet tube, although we suspect that it would. In any case, with purely subsonic (unchoked) flows at both extreme values of the parameters  $\sigma_t$  and  $\sigma_e$ , it appears probable that both an upper and a lower choking boundary in the ( $\sigma_t$  vs.  $\sigma_e$ ) space would be present once some choked case at some intermediate values of  $\sigma_t$  and  $\sigma_e$  has been demonstrated.

The inlet tube is made of a new material "Vylcor" whose fundamental properties are not known. This lack of fundamental data is not significant, however, since we are interested not in the accommodation coefficients of the "clean" surface of this material, but of a contaminated surface

with some uncertain adsorbed gas layer on it. Even if the tube was thoroughly degased during the prolonged orbital flight of the shuttle, it would have acquired its adsorbed gas layer along its descending trajectory and/or through previous sampling for SUMS measurements. It is this uncertain adsorbed layer that plays the crucial role in determining these accommodation coefficients. Under the circumstances, we have to emphasize in our parametric study the qualitative rather than the quantitative, aspects how the  $\sigma_e$  and  $\sigma_t$  will affect the internal flow and the fluxes out of the tube. The possible presence of choking boundary is clearly our greatest concern.

We present in the following selected computed results to illustrate various points. The abscissa indicates the downstream length  $x$  expressed in terms of the number of tube diameter. The ordinate  $Y$  (please note the change of scales in different graphs) designates the values given by the points on the different curves. Each curve is marked by  $N = 1, 2, 3$  etc. to mean  $\beta$ , the mass flux  $DU$  the stream thrust  $p + DU^2$  etc. (with  $p = DT$ ) as are designated in the legend of each figure. These curves are plotted by computer of the results as computed for each case.

Figure 1 illustrates the results of the ideal case of

$$\sigma_e = \sigma_t = 0.$$

Note the nearly exponential decay of the mole fraction  $\beta$  to essentially zero in 20 - 30 diameter tube lengths. Choking results if  $\sigma_e$  is increased to 0.05.

Figure 2 and 3 give typical distributions of unchoked flow properties with  $\sigma_e = 0.05$ ;  $\sigma_t = 0.05$  and 0.20. Note the steep drop of  $\beta$  to essentially zero in 5 to 10 tube diameters. The erratic variations within the first two to three diameters are likely numerical transients due to inherent inconsistencies in the enforced inlet data. If  $\sigma_t$  should be increase to 0.40

with  $\sigma_e = 0.05$ , the flow became choked as the mean velocity became negative in the downstream end of the tube. Figures 4 and 5 are further illustrations of the unchoked flows

at  $\sigma_e = 0.10$      $\sigma_t = 0.40$

and  $\sigma_e = 0.10$      $\sigma_t = 0.80$

The case with  $\sigma_e = 0.10$  and  $\sigma_t = 0.60$  was choked. These results demonstrate the presence of choked internal flow at some intermediate region in the  $(\sigma_e, \sigma_t)$  map and the opposing role of increasing  $\sigma_t$  and  $\sigma_e$ . Similarly at  $\sigma_e = 0.60$ , the flow is choked with  $\sigma_t = 0.30$  but unchoked at  $\sigma_t = 0.20$  and  $\sigma_t = 0.80$ . At  $\sigma_e = 0.40$ , the flow is not choked with  $\sigma_t = 0.40$  but choked with  $\sigma_t = 0.60$ .

Figure 6 is a cross plot of the stream thrust  $p + \rho u^2$  for the computed results at  $\sigma_t = 0.20$  with  $\sigma_e$  varying from 0.05 to 0.60. This figure suggests the relative insignificant role of  $\sigma_e$  in determining the stream thrust in the downstream half of the tube. If the stream thrust at the tube exit should be the physical quantity that determines the change of the pressure in the reservoir, we tend to suggest that the accommodation coefficient of tangential momentum at the tube wall is the primary parameter of importance, so long as the internal flow is not choked. The role of the thermal accommodation coefficient appears to be limited to the choke boundary. Figure 7 illustrates the variation of stream thrust along the tube when  $\sigma_t$  varies while  $\sigma_e = 0.05$  is kept constant. The stream thrust at the tube exit appears to be quite sensitive to the magnitudes of  $\sigma_t$ . This illustration not only reinforces the relative importance of  $\sigma_t$  (over  $\sigma_e$ ) for unchoked flow, but also indicates the extent of sensitivity of the outflux to the small uncertainties in the numerical magnitudes of  $\sigma_t$ .

More computations need be performed to evaluate the influence of the

variation of  $\beta$ ,  $u$  and  $T$  over the SUMS Inlet on the internal flow solution. We are especially concerned about the variation of choking boundary ( $\sigma_e$ ,  $\sigma_t$ ) with  $\beta$ .

The computation given above were carried out with the simple forward time centered space algorithm with time step  $\Delta t = 1$  i.e.  $D/U_\infty \sim 0.3 \times 10^{-6}$  sec. the results given above were computed at  $10^4 \Delta t$  i.e. about 3 millsec after the valve was open. The CPU time required for computing each case is about 20 sec. of IBM 3081. Downstream extrapolation condition is used in the space differentiation at the tube exit. The flow field is still evolving at  $10^4$  steps with perceptible quantitative changes in the next  $10^4$  steps. If the reservoir should respond to variations of millisecc characteristic time, for example, when the SUMS Inlet tube remains open while sampling is controlled by valves further down stream, it may be necessary to determine the transfer function of the tube exit flux to the slowly varying quasi-steady reservoir conditions. The longtime or quasi-steady behavior and other attributes of our unchoked internal flow solution are discussed in Appendix 3, a reprint of paper in the 11th International Conference on Numerical Methods in Fluid Dynamics, at Williamsburg, VA., in 1988 to be published by Springer-Verlag as a volume of Lecture Notes in Physics series. The Fortran program of the computations is enclosed here as Appendix 4.

If the inlet should be choked, the SUMS Inlet condition will have to be altered, either locally or globally, depending on how the external flow will respond. In either case, the internal flow solution will likely be importantly affected by the variation of  $\beta_0$ . Then uncertainty in the evaluation of  $\beta_0$  from the local distribution function(s)  $f_s(u_t)$  and  $f_s(u_n)$  provided by the DSMC solutions cannot be tolerated. This is why the external flow solution by DSMC Method must be improved as to its internal consistency and quantitative accuracy or the external flow solution by the present beam method or other kinetic



formulation must be developed.

$$L1 = DU = 0.48$$

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$$\beta = \beta_0 = 0.37$$

$$\beta = \tau = 11$$

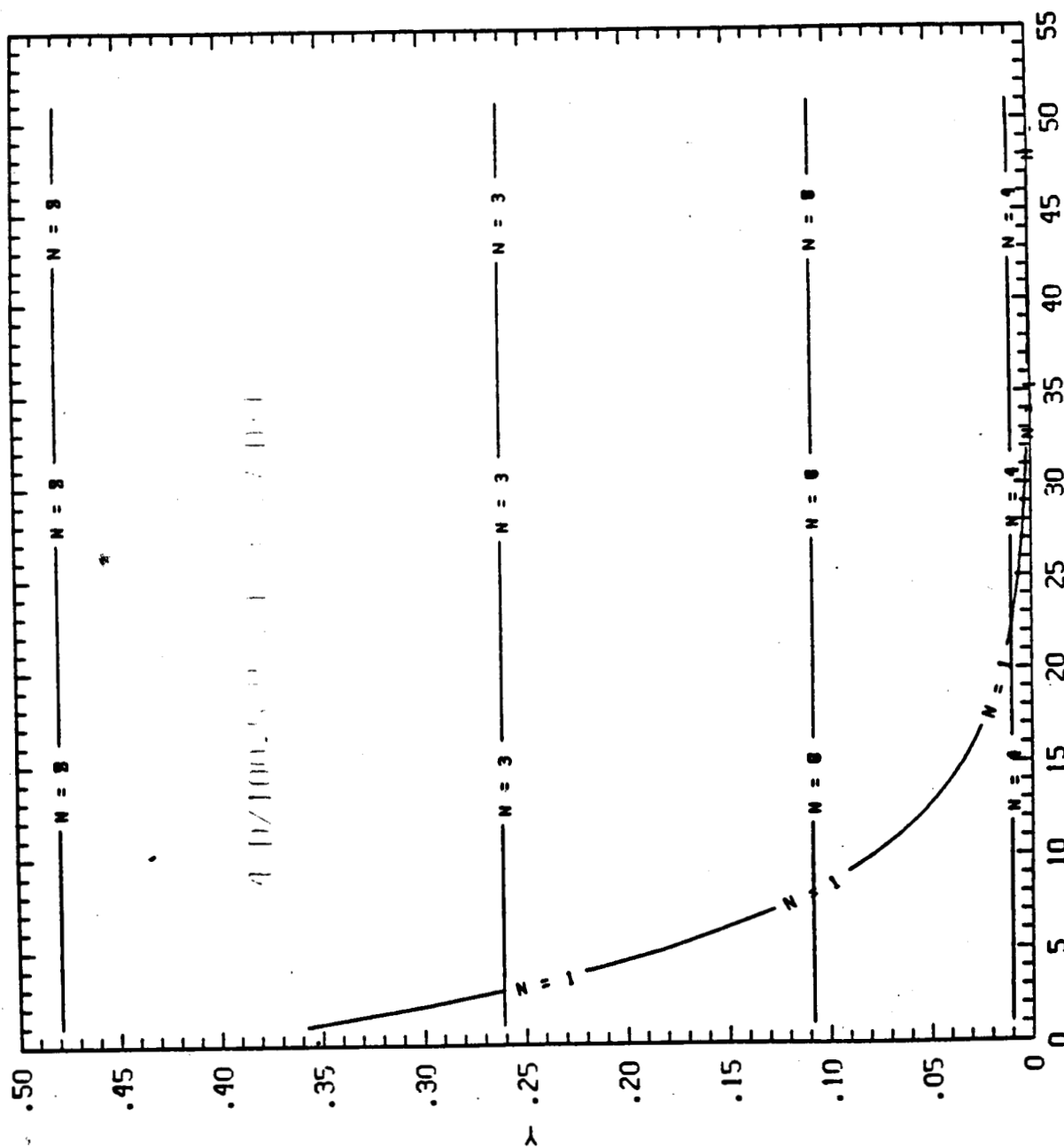
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$$N = 5$$

$$N = 1$$

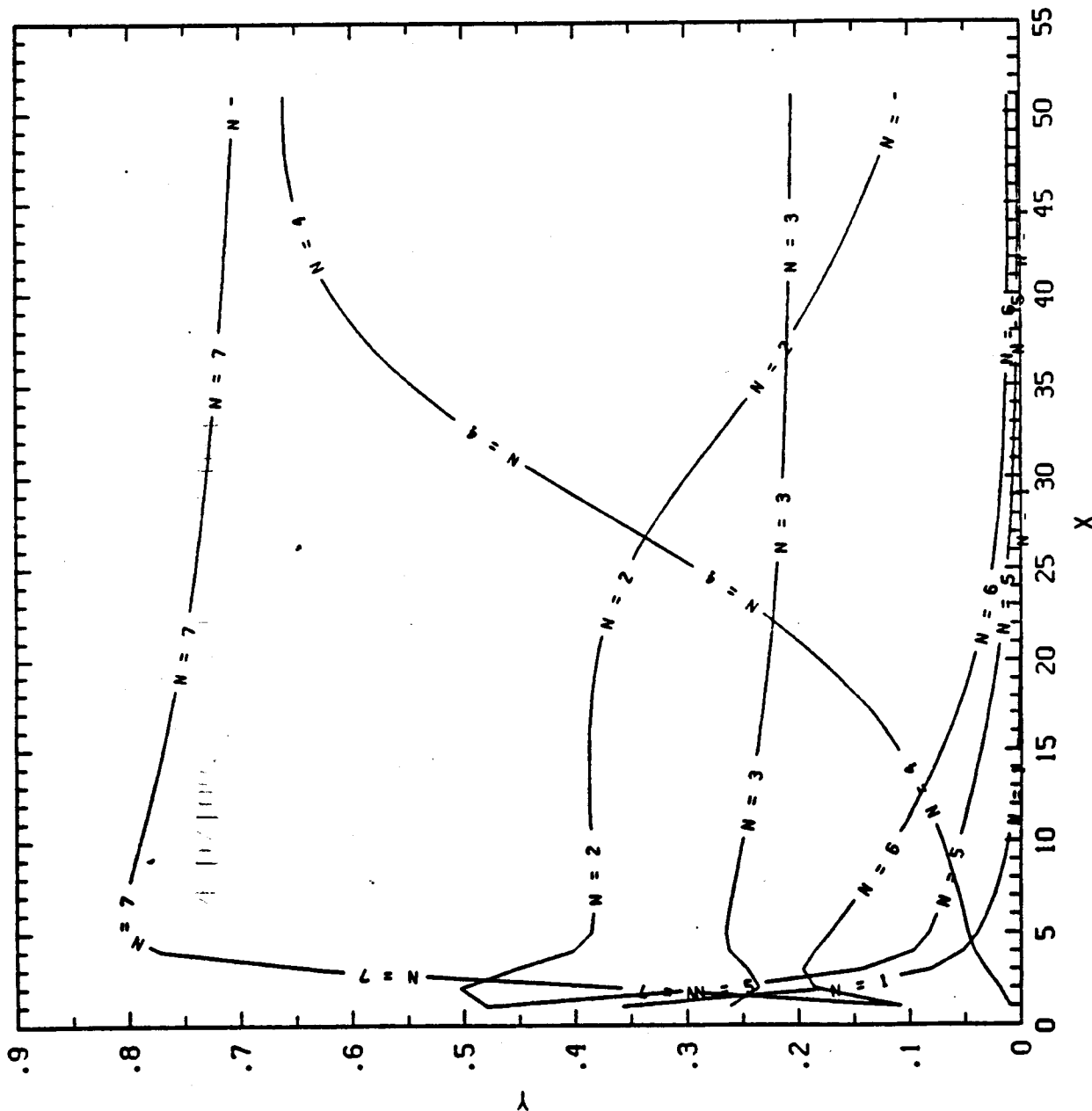
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$$N = 4$$



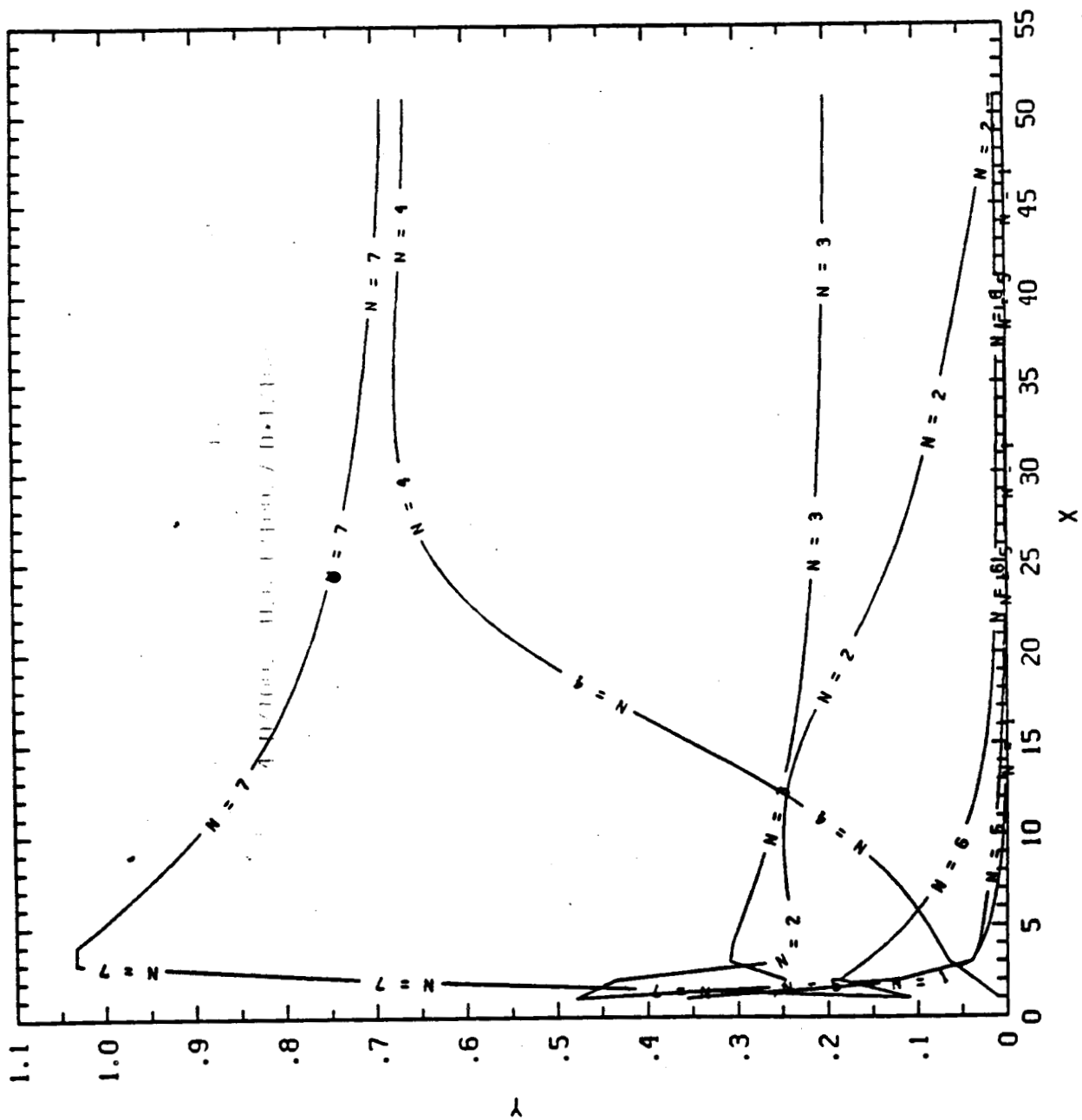
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4-D/100, 5-U, 6-T/100, 7-D\*T/100



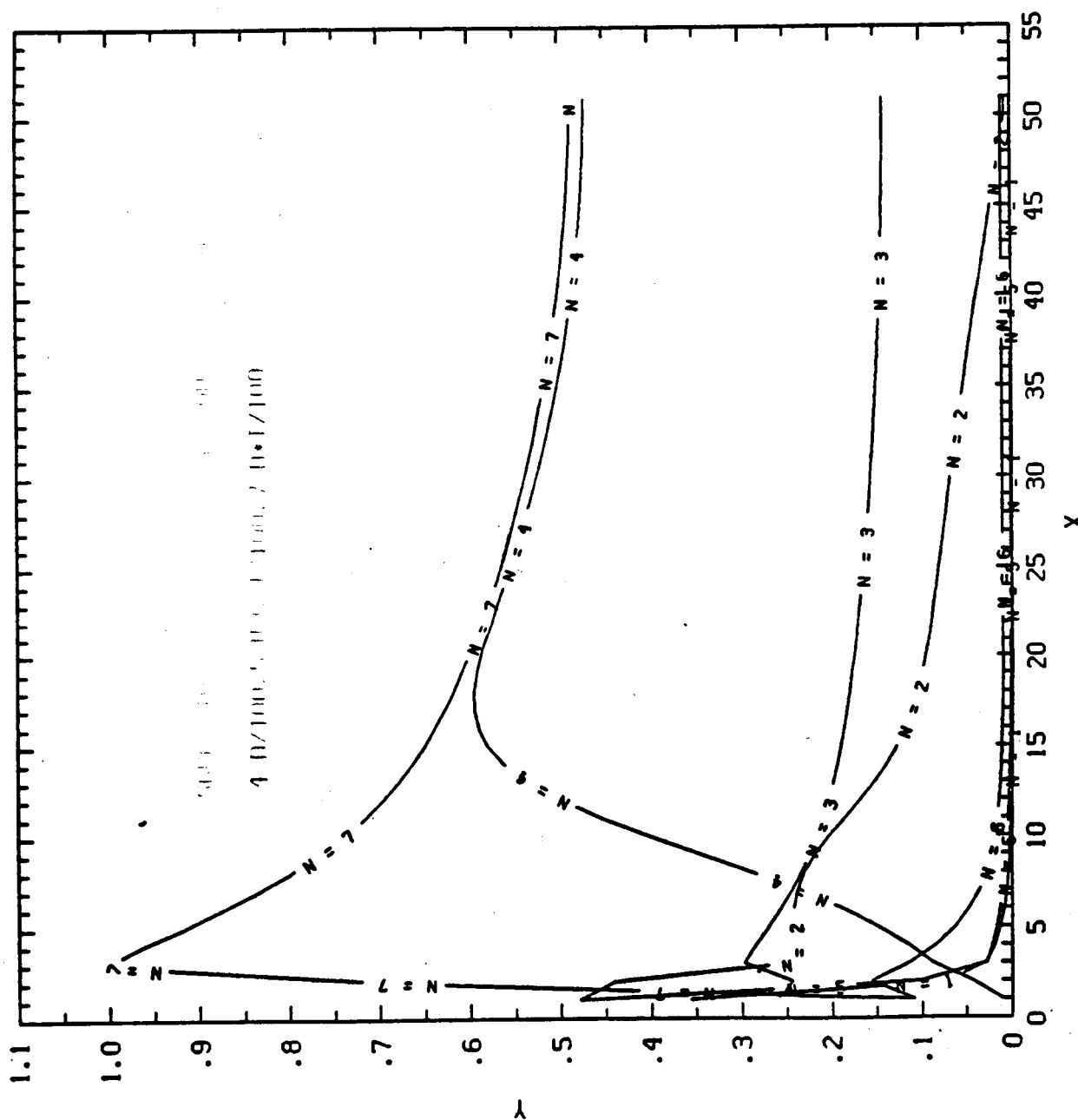
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4-D/100,5-U,6-T/100,7-D#T/100



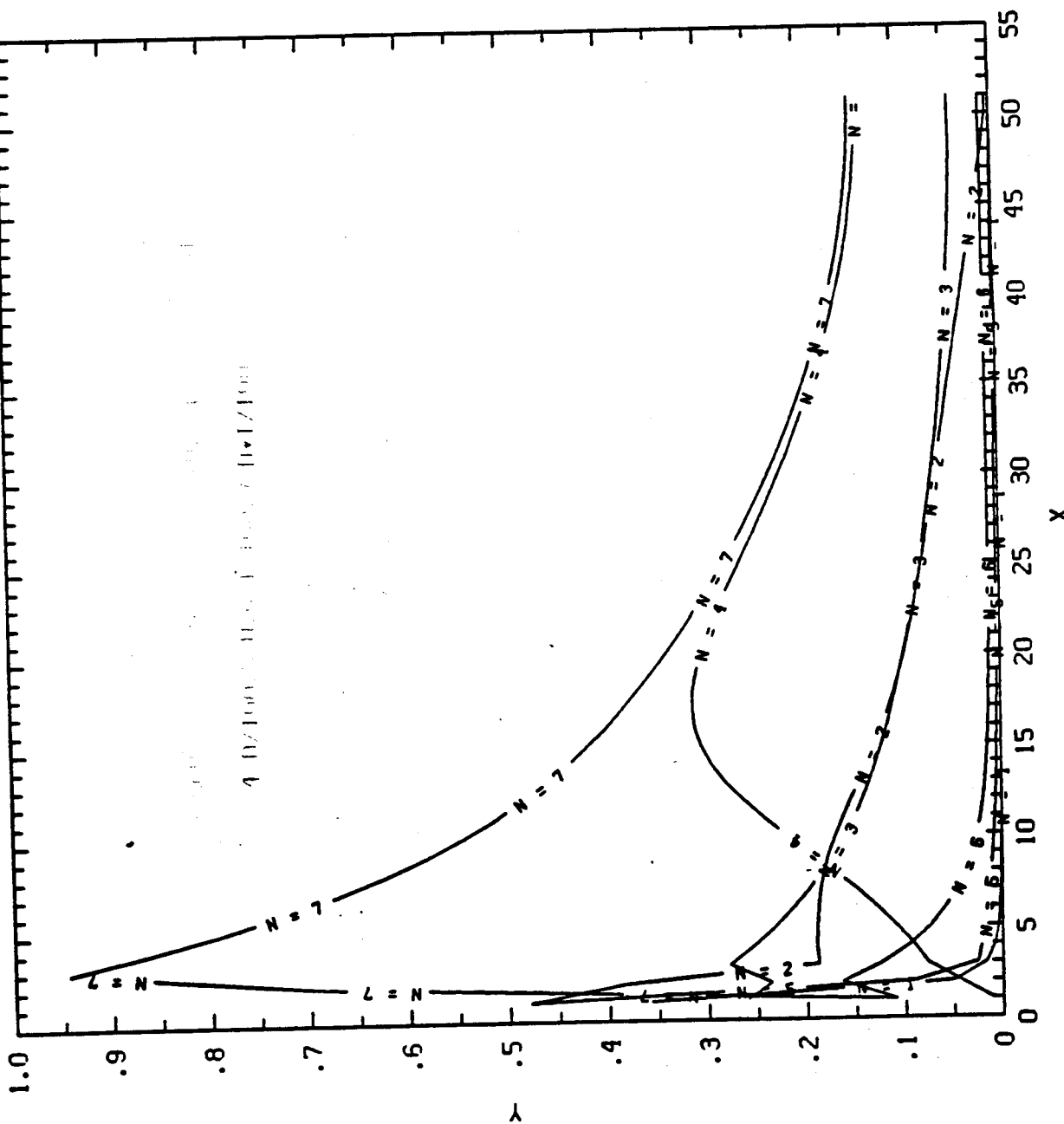
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4-D/100,5-U,6-T/100,7-D\*7/100



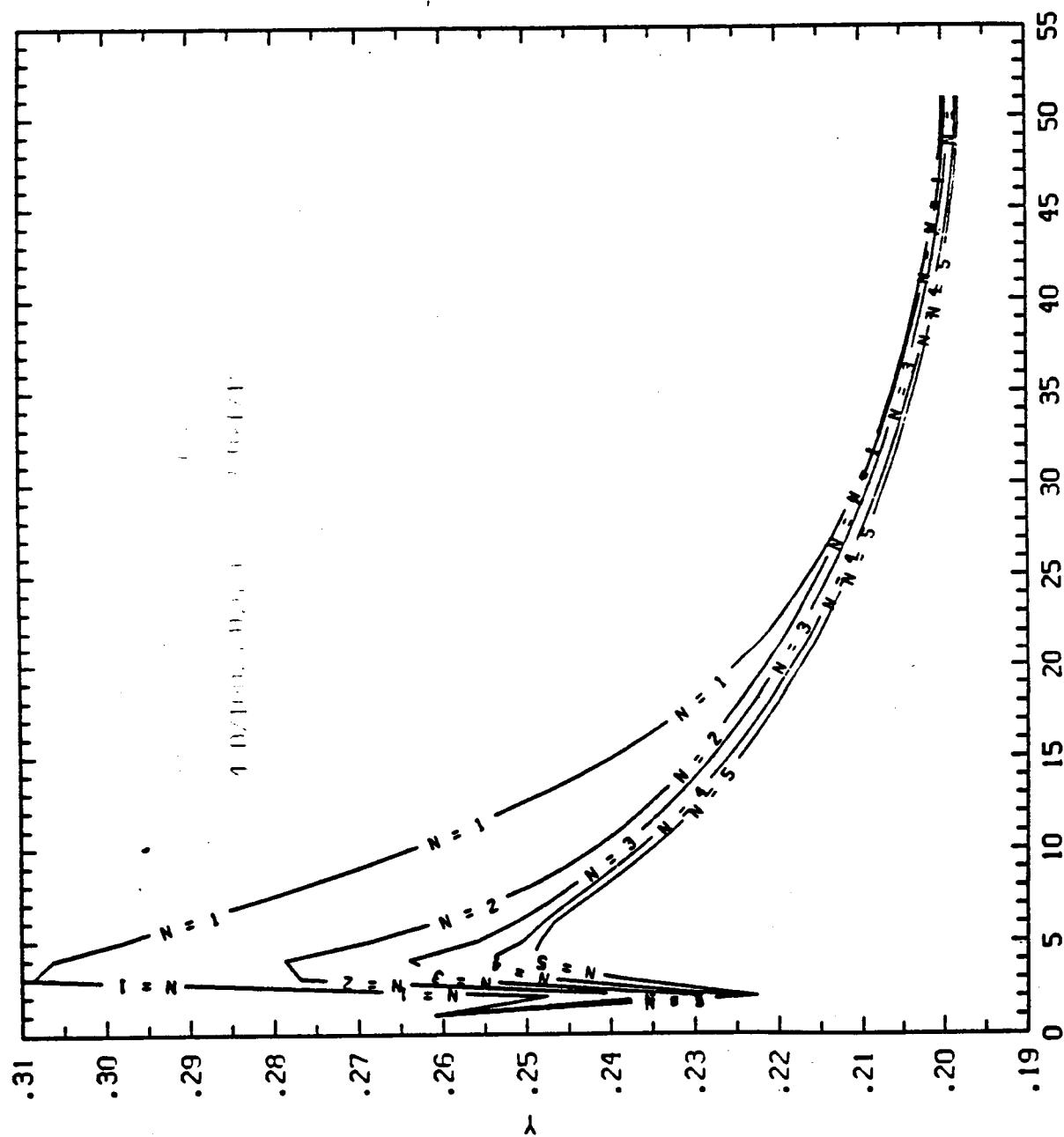
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4-D/100, 5-U, 6-T/100, 7-D\*T/100



SGME=.10, SGMT=.80 1-BETA, 2-DU, 3-DU\*2+P

4-D/100, 5-U, 6-T/100, 7-D\*1/100

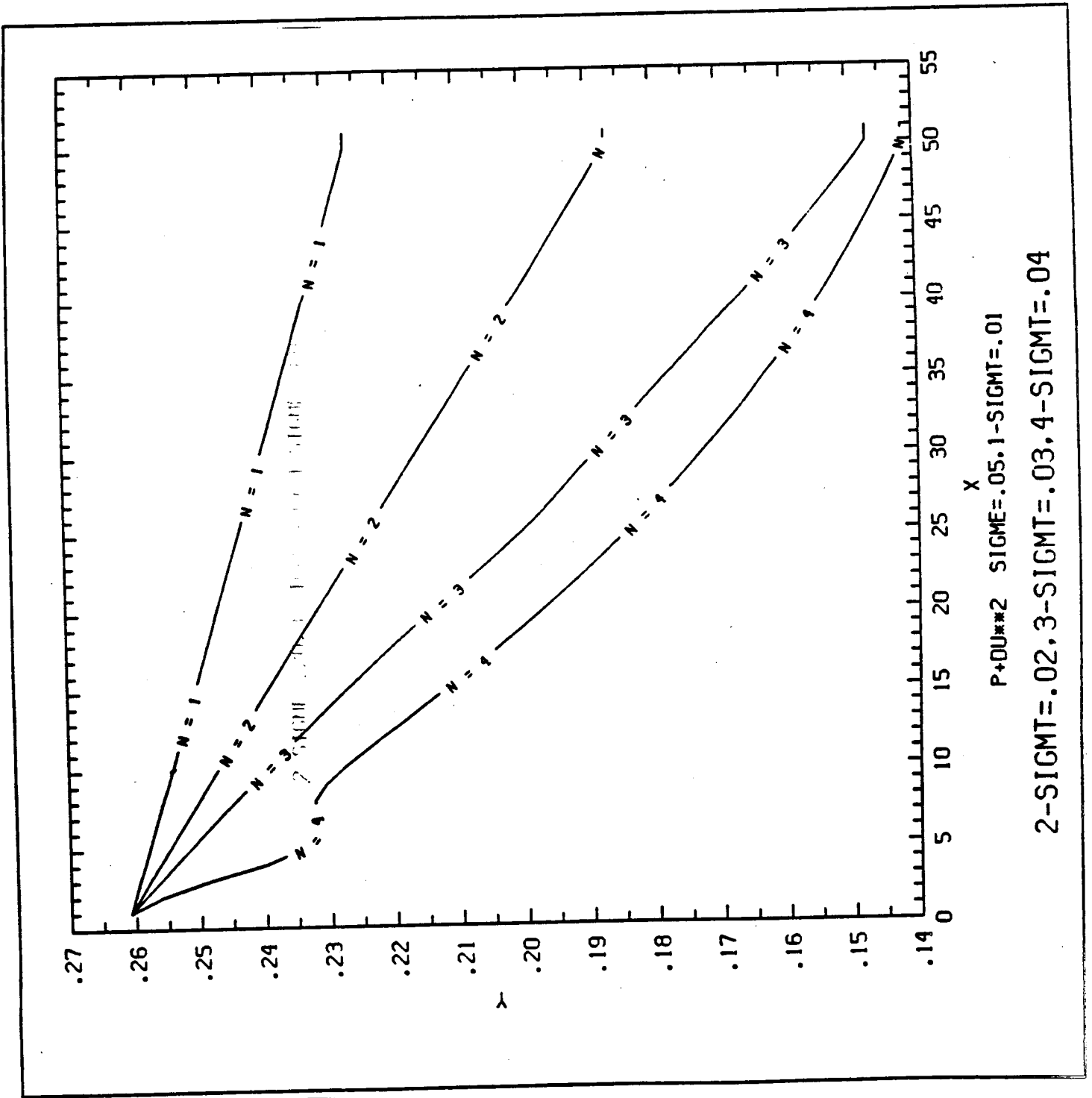


$P+DU=2$  SIGMT=.20.1--SIGME=.05

2-SIGME=.20.3-SIGME=.40.4-SIGME=.60

10.16.

7





## COMPUTATION OF RAREFIED HYPERSONIC FLOWS

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Our interest in lifting maneuverable hypersonic vehicles in orbital transfer or cruise calls for the lift-drag aerodynamic characteristics at altitudes much above 40 Km where the gaseous mean free path  $\lambda$  is not small. The "merged layer" formulation<sup>(1)</sup> of the Navier-Stokes system is no longer adequate. For free molecular flows with the gas-gas molecular interaction neglected entirely, we have the Newtonian approximation,<sup>(2)</sup> where the aerodynamic pressure on a surface is locally determined by the surface angle  $\phi$  as  $\sim \rho U^2 \sin^2 \phi$ . This turns out to be an excellent approximation in the Continuum Limit, especially after some minor empirical corrections. With little difference of surface pressure in both the free molecular and the continuum limits, it is widely presumed that the pressure and the force coefficients on a surface vary smoothly and "monotonically" through the transition range. This is adopted in the analysis of the vehicle acceleration data of some early Shuttle flights<sup>(3)(4)</sup>. An anomalous (~50%) deviation of atmospheric density from the standard atmosphere around 120Km was revealed. Thus SUMS program was established to study it. Air sample was taken from Shuttle surface through a short straight tube, and led to an instrument package with a Mass Spectrometer which has been calibrated with some quasi-steady gas reservoir conditions. For interpreting the data, the "reservoir" condition has to be related to the gas states entering the tube (Internal Flow problem) and then to the undisturbed atmosphere flowing over the Shuttle (External Flow Problem). This is analogous to the Rayleigh probe problem, fundamental to the measurements in continuum supersonic gas dynamics. The rarefied gas in both the internal and the external flow problems is highly "Nonequilibrium" with molecular distribution function governed by the Boltzmann equation whose solution is difficult. The popular Direct Simulation Monte Carlo Method (DSMC), does not pretend to solve the Boltzmann Equation<sup>(6,7)</sup> but to simulate the evolution of the distribution function with a much smaller ensemble of Monte Carlo Particles. A smooth, monotonic variation of the drag coefficient from the continuum to the free molecular state for the external flow was obtained with double peaked distribution functions over SUMS inlet; but no meaningful internal flow

solution<sup>(7)(8)</sup> can be generated despite free adjustments of many numerical and physical parameters.

We cannot help recalling the fundamental deficiencies of the DSMC that repeated sampling in a small computational cell is incompatible with the physics of a hypersonic rarefied flow where  $M K_N \gg 1$  (not  $\ll 1$ ). For such a non-equilibrium system, the central limit theorem and the principle of detailed balance are inapplicable. The DSMC computations let many collisions among the randomly chosen pair of Monte Carlo Particles (MCP) to proceed for some fixed, small convective  $\Delta t_c \ll \Delta x/U$ , chosen in such a manner that the molecules within each computational cell will not cross the cell boundary. When each such MCP is identified as an individual molecule<sup>(9)</sup>, the free flight time of such molecules will be  $\lambda/c$ . In order to have the many collisions as the central limit theorem calls for, we should have  $\lambda/c \ll \Delta t_c \ll \Delta x/U \ll D/U$ ; i.e.  $M K_N \ll 1$  contrary to the condition of a hypersonic rarefied flow with  $M K_N \gg 1$ . A plausible alternative to avoid such a contradiction is to recognize each MAC as a micro-ensemble of molecules, (denied by the popular notion of DSMC<sup>(9)</sup>) whose collective interaction can be compatible with  $M K_N \gg 1$ . Moreover, the collision cross section of such collective interactions can involve many "internal degrees" of freedom, accompanied by many physical constants, desired and proposed<sup>(6)</sup> for DSMC to reproduce better the physical results. Such DSMC will surely provide some reasonable external flow solution once we know what it should be. For the internal flow problems, we have to consider some alternative approach, however.

The double peaked molecular distribution function  $f = f_1 + f_2$  consists of a nearly mono-energetic peak of incoming molecules  $f_1$  and a broad spectrum of scattered molecules  $f_2$  with mole fractions  $\beta$  and  $1-\beta$  respectively. The mean values of each beam defined through Maxwellian fits of  $f_1$  and  $f_2$ , are governed by the integrated moment equations of Boltzmann over their respective velocity spaces. They are like Navier-Stokes, one set for each beam with stress tensor  $\tau_{ij}$  and heat transfer vector  $q_i$  resulting from (i) the departure of  $f_1$  or  $f_2$  from Maxwellian and (ii) the inter-beam collisions. If beam 1 molecules are identified as those undisturbed molecules the equations system for beam 1 gives the rate of change of its population  $\rho_1 = \rho\beta$ . We then define the mean properties of the mixture as  $\rho = \rho_1 + \rho_2$ ,  $p = p_1 + p_2$ ,  $T = \beta T_1 + (1-\beta)T_2$  and  $u = \beta u_1 + (1-\beta)u_2$ ; and replace  $\rho_2 = \rho - \rho_1$  etc. in the N. S. like system for beam 2. For the flow of such a hypersonic rarefied gas mixture through a straight-inlet tube, we can

integrate across the tube to obtain:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \quad (1)$$

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial}{\partial x} (\rho u^2 + p) = -4 \tau_w \quad (2)$$

$$\frac{\partial (\rho e)}{\partial t} + \frac{\partial}{\partial x} (\rho u e) + p \frac{\partial u}{\partial x} = -4 \dot{q}_w \quad (3)$$

where  $u$  is the mean velocity along the tube. Our gas-surface interaction model gives:

$$\left( \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} \right) (\rho \beta) = \rho \beta C_1 \quad (4)$$

$$\tau_w = \frac{1}{4} \rho \sigma_t [\beta C_1 U_1 + (1-\beta) C_2 u_2] \quad (5)$$

$$\begin{aligned} \dot{q}_w = \frac{1}{4} \rho \sigma_e \left[ \beta C_1 \left( e_1 + \frac{(u_1)^2}{2} \right) - \left( e_w + \frac{(1-\sigma_t)^2 (u_1)^2}{2} \right) \right] \\ + (1-\beta) C_2 \left( e_2 + \frac{(u_2)^2}{2} \right) - e_w + \left( \frac{(1-\sigma_t)^2 (u_2)^2}{2} \right) \end{aligned} \quad (6)$$

for the evolution of  $\beta$ , the wall friction  $\tau_w$  and the wall heat transfer vector  $\dot{q}_w$ .  $\sigma_t$  and  $\sigma_e$  are the accommodation coefficients of the tangential momentum and the total energy respectively.

The gas molecules collide almost exclusively with the molecules in the adsorbed gaseous layer over the tube wall to establish an approximate equilibrium flow with varying mean flow properties along the tube. Their evolution is analogous to that of one dimensional continuum gas flow in a tube with friction and heat transfer. As an initial value problem, the evolution can be treated first with a vacuum reservoir condition in the downstream. The residual gas at some low pressure in the reservoir will generate a counter flow from the exit of the tube (reservoir) toward the inlet, without interfering with the free molecular inflow. Therefore, we solve equations system (1)-(6) for flows into a "vacuum reservoir", with the back flow from the reservoir to be superposed separately.

We used explicit, forward time, centered space differencing in terms of the latest available data to discretize (1) - (4). Figures 1, 2 and 3 give some typical results of the variations of different mean flow properties along the tube at 5000 time steps  $\Delta t$  for different fixed, constant values of the

accommodation coefficients  $\sigma_t$  and  $\sigma_e$ .  $\Delta t = D/U \sim 10^{-7}$  sec. for the reference velocity  $U$  to travel the tube diameter  $D$ . The tube was filled with the inlet gas before opening the tube exit. As illustrated in Fig. 4 different initial conditions in the tube give reproducible results after the first few hundred time steps ( $\delta t < 10^{-4}$  sec). A steady state is reached at  $10 \sim 5 \times 10^{-3}$  sec. with zero mean flow velocity and some maximum pressure at the tube exit (Figs. 5,6), expanding freely into the vacuum reservoir with an efflux equal to the influx at the tube inlet. This steady flow condition of the gas at the tube exit expanding freely into a "vacuum" reservoir and the evolution of the gaseous flow within the tube toward this steady state, depend on the accommodation coefficients  $\sigma_t$  and  $\sigma_e$  and the temperature distribution along the tube wall. They are independent of the rarefied reservoir conditions so long as a "Steady State" is reached.

There is a maximum limit of the steady state mass influx into a given tube, beyond which the tube will become "choked" before reaching a steady state of lower mass flux into the vacuum reservoir. The reduction of the influx is accomplished by the generation of upstream propagating pressure waves which will eventually pop out of the tube to alter the external flow over SUMS inlet. This phenomenon is preceded by the occurrence of negative local mean velocity somewhere in the tube. We adopted this latter criterion of imminent choking to define a choking boundary in the  $\sigma_t$  and  $\sigma_e$  space from our computed results with a given wall temperature  $T_w$  distribution and a given tube inlet condition. This boundary defines the maximum steady mass flux that can be pushed through the tube into a vacuum reservoir. When the reservoir contains some low pressure gas it will generate a counter flow out of the inlet tube, with the maximum steady state mass influx correspondingly reduced. Thus the matching of this internal flow solution with the external flow solution over SUMS inlet and with the dynamic characteristics of the instrument package in reducing the SUMS data is somewhat more complicated. This work is sponsored by NASA Langley under Contract No. NAS1 17234. The author thanks Mr. Y. W. Ma and Ms. Ann Bourlioux for carrying out the computations.

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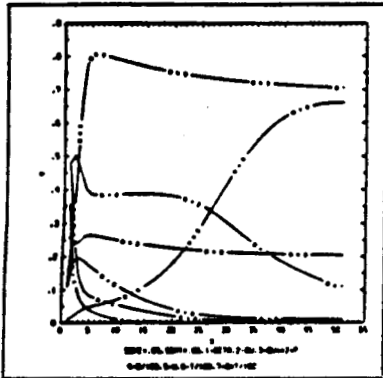


Fig. 1

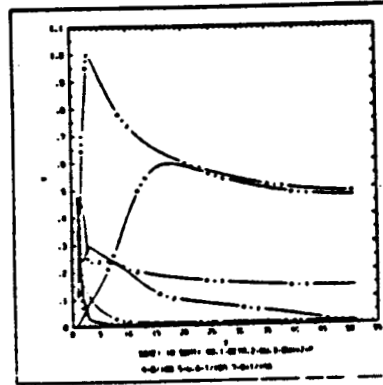


Fig. 2

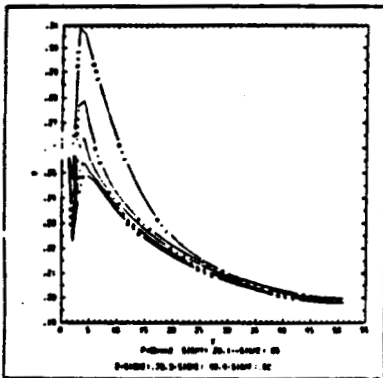


Fig. 3

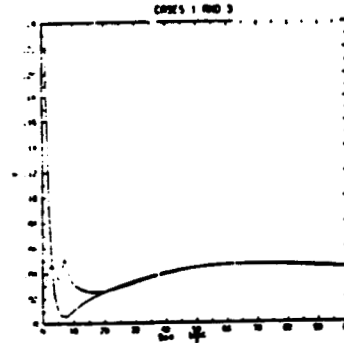


Fig. 4

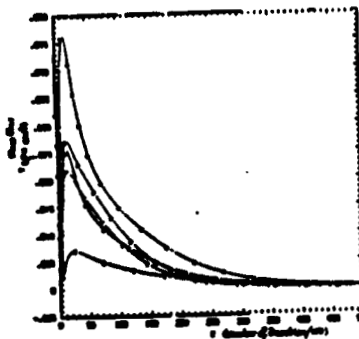


Fig. 5

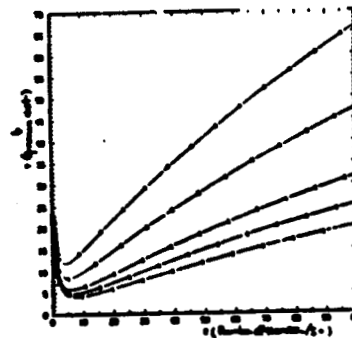


Fig. 6

APPENDIX 4

Fortran Program for Internal Flow Solution

```

*****
c      1-d pipe flow test
*****
c      dimension d(201),u(201),t(201),r(10,201),rg(4,201),p(201),af1(201)
c      % .af(20,201),u2(201),t2(201),c2(201),b(201)
-----
c      the following data must be given in computation
c      y1      : yield parameter
c      y2      : yield parameter
c      sgme     : accommodation coefficient
c      sgmt     : accommodation coefficient
c      qg       : angle between tube and body axes
c      qOO      : angle of attack
c      am       : free mach number
c      tOO      : temperature at infinity
c      xlength  : nondimensional length of the tube
c      usnp     : mean velocity of the normal particle flux incident
c               : onto the surface over cOO
c      ustp     : slip velocity      over cOO
c               : where cOO is sound speed at infinity
c      tsp      : spread of first broad peak
c      tt1      : spread of narrow peak
c      tt2      : spread of broad peak
c      xl       : left end of interval on which the distribution
c               : function is defined
c      xr       : right end of interval of distribution func. definition
c               : xl and xr are needed for definition of bO
c      in       : total mesh points
c      dtx      : time increment/space increment
c      nn10     : print nn10 times results
c      nn11     : print results after nn11 time steps
c      mshck    : = 0 with given entrance conditions
c               : = 1 with post shock entrance conditions
c      v1       : center of narrow peak for vt
c      v2       : center of broad peak for vt
c      a1       : coefficient of distribution function for narrow peak vt
c      a2       : coefficient of distribution function for broad peak vt
c      sgmi,j   : sgme,sgmt
c               : pressure of free stream condition
c      bbb      : coefficient in equation for computing beta
-----
c      open(unit=7, file='final', form='formatted')
c      open(unit=8, file='hist', form='formatted')
c      open(unit=4, file='input', form='formatted')
c
c      pi = acos(-1.)
c      sgme = .10
c      sgmt = .80
c      qg   = 60
c      qOO  = 32
c      y1   = 1.
c      u2   = 1.
c      in   = 51
c      dtx  = 1.
c      nn10 = 100
c      nn11 = 5
c      nn10 = 100
c      nn11 = 40
c      mshck = 0
c      tab = 1

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c      t00 = 304.
c      xlength = 8.7/.235
c      usnp = 4.
c      ustp = 1.
c      tsp = 10.
c      read(4,9050) usnp,ustp,tsp
9050 format(3(1x,f4.1))
c      usnp0 = usnp
c      ustp0 = ustp
c      tt1 = 3.3484
c      tt2 = 10.615
c      x1 = -12.
c      xr = 14.
c      v1 = 8.2
c      v2 = 1.
c      a1 = .103
c      a2 = .104
c
c      -----
c      fnsh0 = 10.
c      c00 = 1./am
c      usnp = usnp*c00
c      ustp = ustp*c00
c
c      -----
c      tt1, tt2, x1, xr, are needed for computing b0
c      tt1 : spread of narrow beam for u(n)
c      tt2 : spread of broad beam for u(n)
c      x1 : left end of interval on which the distribution function
c           is defined
c      xr : right end of interval
c
c      -----
c      call bet0(b0,in,tt1,tt2,x1,xr,v1,v2,a1,a2)
c      write(6,9000)b0
9000 format(1x,'bet0 = .e12.5)
c      alf0 = 2.0
c      dx = xlength/(in-1)
c      ra = 1/am**2
c      p0 = ra/1.4
c      cv = p0/.4
c      cp = cv*1.4
c      dtx2 = dtx/2
c      dt = dtx*dx
c      in1 = in-1
c      qg = qg*pi/180.
c      q00 = q00*pi/180.
c      ym1 = y1-1
c      ym2 = y2-1
c      sgm12 = (1-sgmt)**2/2
c      qsi = qg-q00
c      uts = sin(qsi)
c      u10 = cos(qsi)
c      t10 = 1.+uts**2/(2*cp)
c      u20 = usnp
c      t20 = tsp+ustp**2/(2*cp)
c      uavg = b0*u10*(1-b0)+u20
c      vavg = b0*uts*(1-b0)+ustp
c      tavg = b0*t10*(1-b0)+t20
c      sngspd = sqrt(tavg)/am
c      amavg = (vavg**2+sngspd**2)/sngspd**2
c      cptr = 1+p0*(1-2*cos(5/6)*.5**2/2-3*am**2/2-.4-.4/2-.4)**2*.5-1)
c      pavg = cptr/(cos(qsi)**2/A+p0)
c      ra = 2.4*am**2*(1-4*am**2/2)
c      t1 = b0*(t10*(1-b0)+t20)
c      j02 = 1-b0

```



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nstep = 0
do 50 nn0 = 1, nn10
do 60 nn1 = 1, nn11
call omg(in, am, dtx, d, u, t, af)
call rght2(in, dtx, p0, d, u, t, r, af, rg, b, u10)
call rght0(in, dt, y1c10, y2, ym2, am, qw2, qcl, cu10, qw1, sgm12, cv,
% d, u2, t2, c2, b, rg, r, sgmt, sgme, dx, c10, bbb)
c call split1(in, dtx2, af, u, alf0)
c call ip1slv(in, am, dtx, d, u, t, af, rg, cv, alf0, b, u10)
do 15 i = 2, in1
b(i) = rg(4, i) + d(i) * b(i)
t(i) = rg(3, i) + d(i) * (cv * t(i) + u(i) ** 2 / 2)
u(i) = rg(2, i) + d(i) * u(i)
d(i) = rg(1, i) + d(i)
b(i) = b(i) / d(i)
u(i) = u(i) / d(i)
t(i) = (t(i) / d(i) - u(i) ** 2 / 2) / cv
r(1, i) = 1 - b(i)
u2(i) = (u(i) - b(i) * u10) / r(1, i)
t2(i) = (t(i) - b(i) * t10) / r(1, i)
15 continue
c -----
c down stream boundary conditions for explicit portion
c -----
d(in) = d(in1)
u(in) = u(in1)
t(in) = t(in1)
b(in) = b(in1)
u2(in) = u2(in1)
t2(in) = t2(in1)
c -----
nstep = nstep + 1
do 80 i = 1, in
p(i) = d(i) * t(i)
rg(1, i) = u(i) * am / sqrt(abs(t(i)))
rg(2, i) = d(i) * u(i)
rg(3, i) = p(i) * p0 + rg(2, i) * u(i)
20 continue
fnsh1 = rg(3, in)
c if(fnsh0.lt.fnsh1) go to 33
fnsh0 = fnsh1
40 continue
q0 = q00 * 180. / pi
q1 = qg * 180. / pi
c write(6, 92) am, dtx, alf0, y1, y2, sgme, sgmt, nstep
c write(6, 93) q0, q1, t00, u10, uts, t10, u20, t20, mshck, bbb
c if(mshck.eq.0) go to 30
c write(6, 96)
c go to 31
c 30 continue
c write(6, 97)
c 31 continue
write(8, 9550) nstep, rg(2, in), p(in)
9550 format(' nstep=', i5, ', du=', e11, 4, ', p=', e11, 4)
c write(6, 91)
c write(6, 95)
c write(6, 91)
c write(6, 90) (i, d(i), u(i), t(i), p(i), b(i), u2(i), t2(i), rg(1, i),
% rg(2, i), rg(3, i), i = 1, in)
c write(6, 91)
90 format((1x, i3, 10(1x, e10, 3))
91 format(1x, 11(3e10, 1x)
92 format(2x, 2b2e11, 4, 2x, 4b2e11, 4, 2x, 5b2e10, e11, 4, 2x,
% 5b2e11, 4, 2x, 1b2e11, 4, 1x, 5b2e10, e11, 4, 2x,

```

```

      us1 = 1.
      ts1 = 1.
      call shock(am, dd2, u2, tt2, ds2, us2, ts2)
      ds = ds1+ds2
      us = b0*us1+(1-b0)*us2
      ts = b0*ts1+(1-b0)*ts2
      ams = us*am/sqrt(ts)
      ps = p0*ds*ts
      ps0 = ps*(1+.2*ams**2)**3.5
      pavrg = ps0/(1+.2*amavrg)**3.5
      davrg = pavrg/(p0*tavrg)
      d0 = davrg
      d0 = 1.
c-----
c      treatment of entrance condotions:
c      mshck = 0      :      with given entrance conditions
c      mshck = 1      :      with post      shock conditions
c-----
      if(mshck.eq.0) go to 25
      d10 = b0*d0
      call shock(am, d10, u10, t10, ds1, us1, ts1)
      am2 = u20*am/sqrt(t20)
      d20 = (1-b0)*d0
      if(am2.gt.1.) go to 26
      ds2 = d20
      us2 = u20
      ts2 = t20
      go to 27
26      continue
      call shock(am, d20, u20, t20, ds2, us2, ts2)
27      continue
      d0 = ds1+ds2
      b0 = ds1/d0
      u10 = us1
      t10 = ts1
      u20 = us2
      t20 = ts2
25      continue
      c10 = sqrt(t10)/am
      y1 = ym1*c10
      cu10 = c10*u10
      qw1 = c10*(cv*t10+u10**2/2)
      qw2 = y1*c10*sgm12*u10**2
      y1c10 = y1*c10
c-----
c      initial data at t = 0
c-----
      do 20 i = 1, in
      b (i) = b0
      u2(i) = u20
      t2(i) = t20
      d (i) = d0
      u (i) = b(i)*u10+(1-b(i))*u2(i)
      t (i) = b(i)*t10+(1-b(i))*t2(i)
20      continue
c-----
c      read (15) am, dtv, dalf0, y1, y2, sgms, sgmt, nstep,
c      % q0, q1, t00, u10, u1s, c10, u20, t20, bbb
c      read (15) d, u, t, p, u2, t2, rg
c-----
c
      write(6,9450) t00,u10,p0,u20,t20,b0
9450      format(1x, 'T00=',E12.3, ' U10=',E12.3, ' P0=',E12.3, ' U20=',E12.3, ' B0=',E12.3, '

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% 4ht20=, e11. 4, 2x, 6hmsck=, i2, 2x, 4hbbb=, e11. 4)
95 format(1x, 3(1hi), 1x, 10(1hd), 1x, 10(1hu), 1x, 10(1ht), 1x, 10(1hp),
% 1x, 10(1hb), 1x, 5(2hu2), 1x, 5(2ht2), 1x, 10hmacnumber, 1x,
% 5(2hdu), 3x, 7hp+du**2)
96 format(2x, 5(6hshock ))
97 format(2x, 5(9hno shock ))
write(6,*) fnsh1
50 continue

c...
write(7, 9500) tsp, usnp0, ustp0, b0, nstep
9500 format(1x, 'TSP=', f3. 0, ' USNP=', f3. 0, ' USTP=', f3. 1,
& ' BETA0=', f5. 3, ' NSTEP=', i5)
write(7, 91)
write(7, 95)
write(7, 91)
write(7, 90)(i, d(i), u(i), t(i), p(i), b(i), u2(i), t2(i),
& rg(1, i), rg(2, i), rg(3, i), i=1, in)

c...
33 continue
c write(6, 92) am, dtx, alf0, y1, y2, sgme, sgmt, nstep
c write(6, 93) q0, q1, t00, u10, uts, t10, u20, t20, mshck, bbb
c write(6, 91)
c write(6, 95)
c write(6, 91)
c write(6, 90)(i, d(i), u(i), t(i), p(i), b(i), u2(i), t2(i), rg(1, i),
c % rg(2, i), rg(3, i), i = 1, in)
c write (85) am, dtx, alf0, y1, y2, sgme, sgmt, nstep,
c % q0, q1, t00, u10, uts, t10, u20, t20, mshck, bbb
c write (86) d, u, t, p, b, u2, t2, rg
c stop
c end

c*****
c define b0 = (area narrow)/((area narrow)+(area broad))
c t1 : spread of narrow beam
c t2 : spread of broad beam
c x1 : left end of integral
c xr : right end of integral
c-----
subroutine bet0(b0, m, t1, t2, x1, xr, v1, v2, a1, a2)
k1 = m-1
cst1 = 1.4/(2*t1)
cst2 = 1.4/(2*t2)
dz = (xr-x1)/k1
z = x1
arbrw = a1*exp(-cst1*(z-v1)**2)/2
arbrd = a2*exp(-cst2*(z-v2)**2)/2
do 10 k = 2, k1
z = z+dz
arbrw = arbrw+a1*exp(-cst1*(z-v1)**2)
arbrd = arbrd+a2*exp(-cst2*(z-v2)**2)
10 continue
z = z+dz
arbrw = (arbrw+a1*exp(-cst1*(z-v1)**2)/2)*dz
arbrd = (arbrd+a2*exp(-cst2*(z-v2)**2)/2)*dz
b0 = arbrw/(arbrw+arbrd)
return
end

c> *****
c source term treatment
c-----
subroutine rght0(in, dt, y1, t10, y2, ym2, am, qw2, r1, r2, r3, r4, cv, d,
% u2, t2, c2, b, rg, r, sgmt, sgme, dx, c10, bbb)
dimension d(in), u2(in), t2(in), c2(in), b(in), rg(4, in), r(10, in)

```

```

c2(i) = sqrt(abs(t2(i)))/am
r(1,i) = (1-b(i))*c2(i)
r(2,i) = dt*d(i)
rg(1,i) = rg(1,i)+r(2,i)*(b(i)*r1+ym2*r(1,i))
rg(2,i) = rg(2,i)-r(2,i)*(b(i)*r2+r(1,i)*u2(i))*sgmt
rg(3,i) = rg(3,i)-r(2,i)*(b(i)*(r3-qw2-y1c10*ew)+
% r(1,i)*(cv*t2(i)+u2(i)**2/2-y2*(ew+r4*u2(i)**2))*sgme
rg(4,i) = rg(4,i)-r(2,i)*b(i)*c10*bbb
10 continue
return
end
c*****
c      invisid upwind difference for explicit portion
c-----
      subroutine rght2(in,dtx,p0,d,u,t,r,af,rg,b,u10)
      dimension d(in),u(in),t(in),r(10,in),af(20,in),rg(4,in),b(in)
      in1 = in-1
      do 10 i = 1,in
        r(1,i) = d(i)*t(i)*p0
        r(2,i) = d(i)*u(i)
        r(3,i) = r(2,i)*u(i)
        r(4,i) = (r(1,i)/.4+r(3,i)/2)*u(i)
        r(5,i) = af(12,i)*r(1,i)
        r(6,i) = af(13,i)*r(1,i)
        r(7,i) = af(14,i)*r(1,i)
        r(8,i) = r(1,i)*u(i)/2
        r(2,i) = r(2,i)+r(5,i)
        r(3,i) = r(3,i)+r(1,i)/2+r(6,i)
        r(4,i) = r(4,i)+r(8,i)+r(7,i)
        r(6,i) = r(1,i)/2-r(6,i)
        r(7,i) = r(8,i)-r(7,i)
        r(9,i) = d(i)*b(i)*u10
      10 continue
      do 11 i = 2,in1
        rg(1,i) = dtx*(r(2,i-1)-r(2,i)+r(5,i+1)-r(5,i))
        rg(2,i) = dtx*(r(3,i-1)-r(3,i)-r(6,i+1)+r(6,i))
        rg(3,i) = dtx*(r(4,i-1)-r(4,i)-r(7,i+1)+r(7,i))
        rg(4,i) = dtx*(r(9,i-1)-r(9,i))
      11 continue
      return
      end
c*****
      subroutine omg(in,am,dtx,d,u,t,af)
      dimension d(in),u(in),t(in),af(20,in)
      dtx2 = dtx/2
      do 10 i = 1,in
        af( 1,i) = sqrt(abs(t(i)))/am
        af(14,i) = u(i)**2/2
        af(15,i) = af(1,i)**2/.4
        af( 8,i) = .4/af(1,i)
        af( 4,i) = af(14,i)-af(15,i)
        af( 5,i) = -u(i)-af(8,i)*af(14,i)
        af( 6,i) = -u(i)+af(8,i)*af(14,i)
        af( 7,i) = af(8,i)*u(i)
        af( 9,i) = -1/af(15,i)
        af(10,i) = af(9,i)*u(i)
        af(11,i) = af(9,i)*af(14,i)
        af(12,i) = .5/af(1,i)
        af(13,i) = af(12,i)*u(i)
        af(14,i) = (af(14,i)+af(15,i))*af(12,i)
      10 continue
      return
      end

```



```

      u4 = rg(4,1)+r14
      rg(4,j) = b4/dtx2
      call slvpls(i,in,b1,b2,b3,rg(1,i),rg(2,i),rg(3,i),u,af)
      r11 = b1-rg(1,i)
      r12 = b2-rg(2,i)
      r13 = b3-rg(3,i)
      r14 = b4-rg(4,i)
10 continue

c-----
c      treatment of boundary conditions for the implicity portion
c-----
      b1 = rg(1,in1)
      b2 = rg(2,in1)
      b3 = rg(3,in1)
c      b2 = u(in)*b1
c      b3 = (cv*t(in)+u(in)**2/2)*b1
c-----
      call ad1(in,in,b1,b2,b3,r11,r12,r13,dtx2,u,af,alf0)
      do 11 k = 2,in1
        i = in+1-k
        b1 = rg(1,i)-r11
        b2 = rg(2,i)-r12
        b3 = rg(3,i)-r13
        call slvmns(i,in,b1,b2,b3,rg(1,i),rg(2,i),rg(3,i),u,af)
        r11 = rg(1,i)-b1
        r12 = rg(2,i)-b2
        r13 = rg(3,i)-b3
11 continue
      return
      end

c*****
      subroutine shock(am,d0,u0,t0,ds,us,ts)
      am0 = u0*am/sqrt(t0)
      p0 = 1/(1.4*am0**2)
      ps = (1-1/am0**2)/1.2+p0
      ds = (ps+p0/6)/(p0+ps/6)
      us = 1-sqrt((1-1/ds)*(ps-p0))
      ts = ps/(ds*p0)
      ds = ds*d0
      us = us*u0
      ts = ts*t0
      return
      end

c*****

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## Appendix 5.

### *In situ Orbital Experiments of Measuring Surface Accommodation Coefficients*

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#### 1. Introduction

In any methods of predicting forces (both normal and tangential) and heat transfer rates on a surface in a rarefied gas, it is essential to know the "accommodation coefficients" of the surface which relates the mean kinematic and dynamic characteristics of the incident molecules and the reflected molecules for the prevailing surface conditions. In the continuum limit, this formulation with accommodation coefficients should reduce to the continuum conditions of nonslip accompanied by the appropriate viscosity and heat conductivity coefficients. We have little idea what the free molecular limit would be if there should be such a limit. Neither do we have much idea as to their values and their variations in the rarefied continuum transition range. To choose values of such accommodation coefficients so as to predict global results of the limited amount of experimental data of complex flow fields is of little practical significance. It is practically impossible to validate one method vs. any others under the circumstances. There cannot be any predictive methods without knowing these accommodation coefficients. It is essential to collect a sufficient amount of experimental data that will serve to determine these coefficients in some reliable fashion.

The functional forms of the relations between the various properties of the

incident, the reflected and the surface molecules are not well established. The accommodation coefficients as parameters in such functional relations are yet to be defined precisely. Maxwell<sup>(1)</sup> might have suggested a linear relation between the mean properties of reflected molecules and incident molecules. He introduced the notion of the diffused and the specular reflection from a surface that is "rough" or "perfectly smooth", with accommodation coefficients zero or one respectively. A solid surface, however, is always very rough at the atomic or molecular scale although very smooth as a continuum. We hope of course, such accommodation coefficients might be "physical properties" of the incident gas (and/or those of the surface) just as the viscosity coefficient of a dense gas under the model of the gradient diffusion for molecular shear stress following Navier and Stokes. It is disturbing, however, this conventional form of the accommodation coefficients does not appear to be compatible with or reducible to the continuum description of nonslip and gradient type diffusion in the limit. Neither can we visualize how some gradient type diffusion models might be compatible with the free molecular situation. We shall therefore present first a physical model of gas surface interaction, possessing the appropriate limits and with accommodation coefficients introduced within Maxwell's concept. We are unsure if the accommodation coefficients so defined will remain reasonably constant within the transition range as "physical properties" should when evaluated from reliable sets of redundant experiment data. If not so we may have to redefine our accommodation coefficients or to correct our physical model.

Any meaningful experiment should be done in situ i.e. in the actual flight environment of the Hypersonic rarefied gas condition in successive orbits or along the shuttle trajectory for SUMS application. This is because of the uncertainties implicit in the constituent properties of the atmosphere and of the



surface in question. The surface is "Contaminated". We do not know how to specify such a "contaminated" surface for performing the appropriate experiments in laboratory on Earth surface. There are many experimental data of "accommodation coefficients" and of detailed studies of scattering patterns but only for "Carefully cleaned" metallic surfaces and mostly for noble gaseous particles with incident energy considerably above the 1-10 eV range (2,3). It has been generally reported that "contaminated" or "not-thoroughly degassed" surfaces would give meaningless results (presumably highly variable and significantly different). For the SUMS program we need precisely the accommodation coefficients of surfaces specifically contaminated through some uncertain past history and degassed in the not so well known orbital conditions. It is likely that the values of the accommodation coefficients provide the most convenient if not the best specification of the contaminated conditions. This is why we have to consider experiment in Situ; and means of such in Situ experiments are available.

We need a large amount of data for various reasons. The experiment should be as simple as possible, sufficiently repeated and capable of being carried out in situ over a significant range of altitudes and operating conditions. Its reproducibility must be carefully established. We do not know if such coefficients will be little affected by seasonal, and/or geological variations over the globe, and if they will be insensitive to altitudes throughout the free-molecule-continuum transition range. There may be significant effects of transients such as solar flares or solar winds or other electromagnetic storms etc., with serious implications on the dynamics of a vehicle under such transients if not on the "mean values".

## 2. Physical Model of Surface Interaction

We shall describe briefly our model with a crystalline metallic surface although the surface material of interest need not be truly crystalline metallic. Whether the surface material is amorphous, ceramic or truly metallic, the surface is representable by a porous array of atoms some of these may carry their own characteristic electric charges. The important feature is that it is largely "Empty" with a large number of small atoms scattered over the scene, maybe with loose electrons wandering around. Each individual atom is "vibrating" about its mean location. Excepting the detailed arrangements of such particles, we shall tentatively illustrate the surface as a regular lattice of simple structure. The same argument will go through for more complex material structure to suggest the same surface interaction model. We presume that the different material structures will not alter the basic form of the functional relationship, although they may alter the magnitudes of the coefficients in the surface interaction model.

Consider the incidence of a gas molecule onto a "perfectly cleaned" metallic surface. Most probably it will penetrate into the lattice and collide with different lattice molecules successively and lose most of its excess energy. The disturbed lattice molecules (atoms) will restore their respective equilibrium positions while the incident gas molecule wanders through the maze to emerge back to the surface. It cannot escape the surface because it is unlikely to possess the energy necessary to escape the surface potential  $\phi$ , likely of the order of 1 ev. The surface potential exists because of the asymmetry of "mass distribution" across the surface. This surface potential extends no more than the lattice dimension likely  $O(\text{\AA})$ . The incident molecule eventually got trapped in this surface potential  $\phi$ ; and unless excited thermally or otherwise, it cannot

escape. Successive incident molecules become so trapped; and the surface layer becomes sufficiently populated to form an adsorbed layer of gases. This layer weakens the effective surface potential acting on additional incident molecules. Those molecules incident later, may eventually escape themselves or to release some other molecules trapped earlier in the "adsorbed layer". In this manner, a cleaned surface becomes eventually contaminated by the surrounding gas through sufficient long time exposure. This layer of gas molecules trapped in the surface potential becomes eventually the "adsorbed" equilibrium gas layer over the metallic surface with physical constituents varying with the past history of contamination and/or degassing. By necessity, the thin layer of adsorbed gas is densely populated regardless of the nearly vacuum conditions that it may be exposed to at the time or in the near past. In this sense, all the orbital surfaces are contaminated with their own equilibrium adsorbed gas layers.

A gas molecule incident on the contaminated solid surface, will most likely be intercepted by the adsorbed gas layer, rather than to pass through into the atomic arrays of the solid surface. Even if it did penetrate through, it will wander back and become a member of the adsorbed layer eventually. The disturbed adsorbed layer will restore its equilibrium state by emitting one (or more) gas molecule from the adsorbed layer. The relaxation time for the disturbed adsorbed equilibrium layer to return to equilibrium is very small  $O(\hbar/U)$ . The incidence and the emission are almost simultaneous such that the entire process may appear to be a simple "reflection." The incident and the emitted molecules are generally not the same (can indeed be of different species). Surely the average property (ies) of the incident molecules need not be the same as those of the emitted (not really reflected) molecules. The adsorbed gas layer, due to its spatial proximity and to the long time contact with the solid surface, is likely

fully accommodated to the wall thermodynamic conditions, i.e. at rest with the surface and at the same temperature in the mean. While the emitted gas molecules are, among the high energy fraction of the adsorbed molecules, some positive energy accommodation to the wall conditions should be expected. So is for the tangential momentum. The adsorbed molecules with higher energy that escape the adsorbed layer are likely in the vicinity of impact of the impinging gas molecule; and hence, may have received some excess energy of the incident molecule during its passage (or direct interaction) through the adsorbed gas layer. It appears therefore logical to presume that the excess energy and tangential momentum of the emitted gas molecules be related to the excesses of incident gas over the adsorbed wall gas layer molecules.

The suggestion of a linear relationship is clearly an acceptable first approximation without any indications to the contrary. The accommodation coefficient will then stand as the proportional constant  $r_g$  for property  $g$

$$\langle g_e \rangle = (1 - \sigma_g) [\langle g_i \rangle - \langle g_e \rangle]$$

where  $\langle \rangle$  means some statistical average over the ensemble of incident or emitted molecules. We define our accommodation coefficients  $r_g$  only through the mean quantities; although the detailed mechanics of such gas-surface interaction is equally applicable microscopically. The normal momentum flux as a result of such surface dynamics gives rise to the surface pressure distinct from the gas pressure. The net tangential momentum flux (energy flux) lost represents wall friction (heat transfer rate). They are proportional to the accommodation coefficients  $\sigma_t$  (or  $\sigma_e$ ). There is no absolute reason why such a linear relation must prevail, but for Maxwell's suggestion and conventional usage. Its success

is yet to be tested from the data to be gathered from the proposed orbital insitu experiments. Our task is not merely to determine the values of such accommodation coefficients but to test the formulation and the underlying dynamics of the physical model. If need be, better or more detailed models of gas-surface interaction would have to be developed.

The thickness of the adsorbed layer ( $O(\text{\AA})$ ) is so small and the molecular velocities are so large that the relaxation time for the adsorbed layer to maintain its equilibrium is unquestionably negligible compared with any dynamic transit time. The particle yield is likely unity to maintain the equilibrium state. There are, however, uncertainties in the efficiency and extent of momentum and energy transfer from the incident molecules to the adsorbed gas molecules, with the adsorbed gas molecules set into a mean shear motion parallel to the solid surface. In so far as the characteristic Reynolds number is so small, the mean motion of the dense adsorbed gas layer is most likely laminar where the gradient type diffusion model of surface friction prevails. As such the recovery of the continuum limit of gas-surface interaction is largely assured. The free-molecular limit is like Newtonian, but there is no assurance that the accommodation coefficients  $\sigma_t$  and  $\sigma_e$  may be zero or unity implied in the classical Newtonian approximation.

### 3. Hypersonic Dynamics of Rarified-Continuum Transition

According to our model of gas surface interaction, the accommodation coefficients of tangential momentum  $\sigma_t$  and of energy  $\sigma_e$  are formally linearly proportional to the wall friction and heat transfer over a solid surface. To measure  $\sigma_t$  and  $\sigma_e$ , we need (i) the measurements of forces and heat transfer

rate over a simple model surface and (ii) the analytic estimate of the "gas properties" in the proximity of the model surface under the hypersonic flight condition so that we can estimate analytically the friction and the heat transfer rate involved. We address here first the latter problem before discussing the first problem of the details of proposed measurements.

It might appear that the classical or the simple Newtonian hypersonic approximation or the semi-empirical modified Newtonian with centrifugal correction would suffice. We note that such classical Newtonian approximation predicts only the pressure on the windward surface while that on the wake side has to be estimated separately. The tangential stress ( $\sigma_t$ ) and the heat transfer rate ( $\sigma_e$ ) are yet to be estimated with further approximation. The popular DSMC (Direct Simulation Monte Carlo) Method<sup>(4)</sup> has similar problems and more; and it is computation heavy. We have thus developed an analytic formulation for determining the mean flow properties throughout the hypersonic flow field with Knudson number not small,<sup>(5)</sup> explicitly involving  $\sigma_t$  and  $\sigma_e$ .

We hope that for flows over certain simple configurations the gaseous mean flow properties over the solid surface can be more consistently determined, along with explicit relations of wall friction and heat transfer rate with these gaseous mean surface properties through the accommodation coefficients  $\sigma_t$  and  $\sigma_e$ . For the near-Free molecular conditions prevailing around shuttle orbits, we are hopeful of achieving same explicit algebraic relations between these quantities, which will greatly facilitate data processing.

The present formulation is focussed on the solution of mean flow properties based on a one-parameter family of non-equilibrium molecular distribution functions in terms of the mole fraction  $\beta$  of the undisturbed incident hypersonic molecular beam. The population of this undisturbed molecular beam is

monotonically decreasing in its approach to the vehicle surface. They are scattered largely by the diffused beam of molecules emitted or reflected from the vehicle surface. The formulation leads implicitly to the free molecular limit of Newtonian with the appropriate set of "accommodation coefficients" and also to the continuum limit of a bow shock wave standing off from a nonslip vehicle surface. When the Knudson number increases from the continuum range, the shock wave will expand to reach the solid surface. The quasi-continuum description with Hugoniot shock in a rarified gas flow will cease to be valid. The shock profile in the gas may still resemble a part of the hugoniot structure but is incomplete. As the flow Knudson number increases further, undisturbed free stream molecules begin to arrive at the solid surface in appreciable amount ( $\beta > 0$ ) accompanied by the "slip" of gas temperature (or energy) over the wall (surface) temperature. The presence of the slip implies a "jump solution" from the conditions of the surface gas to those of the adsorbed layer in equilibrium with the surface. This latter jump increases in magnitude with higher  $K_N$ . A direct jump from the undisturbed free stream condition ( $\beta = 1$ ) from the proximity of the solid surface to the conditions of the equilibrium adsorbed gas layer on the surface stands as the free molecular Newtonian limit. Details of the transition depend on the surface geometry and the surface condition. Within the present model of gas-surface interaction in equilibrium, the gas properties over the solid surface vary for different vehicles (or solid walls) and under different flight conditions. Even in free molecular limit, the classical Newtonian approximation should be corrected for the surface conditions, in predicting the mean flow properties and the wall friction and heat transfer.

For a general body configurations, the wall friction per unit surface area is presently presumed to be equal to a fraction  $\sigma_t$  (the accommodation

coefficient) of the excess tangential momentum of the surface gas incident on the surface from without the "adsorbed gas layer." This excess can be evaluated from the local surface gas properties ( $\beta_s$ ,  $\rho_s$ ,  $U_s$  and  $T_s$ ) and the local wall temperature  $T_w$  assuming that  $u_w = 0$ ; but all the surface properties are, in general, dependent on the global geometry and the surface conditions from which the scattering beam of molecules originated. Thus all surface quantities, and  $\beta_s$  in particular, depend implicitly on  $\sigma_t$ ,  $\sigma_e$  and  $T_w$  globally. It is only in the free molecular (or Newtonian) limit that  $\beta_s \cong 1$  and  $\rho_s$ ,  $U_s$  and  $T_s$  are the values of the undisturbed incident stream from afar.

Shuttle orbits are sufficiently high (200-300 Km) where the Newtonian approximation is expected to be valid so long as the particular surface is not in the "wake" of the shuttle nose. Thus when the shuttle is maneuvered to expose the instrument package in the "Bay" to the undisturbed free stream, the processing of the data can be greatly facilitated when the wall friction will be truly proportional to  $\sigma_t$  with excess momentum known over the convex surface (i.e. outside the wake). The pressure on the concave side (i.e. within the wake of itself) cannot be accurately estimated but hopefully will be significantly less than that on the convex side of the surface. It appears nevertheless advisable to minimize the associated uncertainties of the wake pressure in the reduction of data by properly designing the experimental set up.

To determine the accommodation coefficients at lower altitudes along shuttle descending trajectory, it may not be convenient to maneuver the shuttle and open the bay in properly positioning the instrument package for such an experiment. To support the instrument package outside the wake with a boom appears cumbersome. To eject the package into the free stream will mean telemetering the data back for processing. To perform the experiment in the bay will require



1  
better estimate of the hypersonic flow environment of the instrument package, where upon, the possibility of laboratory experiments on "recovered" samples from orbital flights may have to be reconsidered. Tentatively we hope that there are no significant changes in the accommodation coefficients with altitudes. Then, the experiment in shuttle orbits will be the most important one. Experiments at lower transitional altitudes may be more complex. We shall therefore devote our experimental considerations here to experiments in shuttle orbits only in the near free molecular condition.

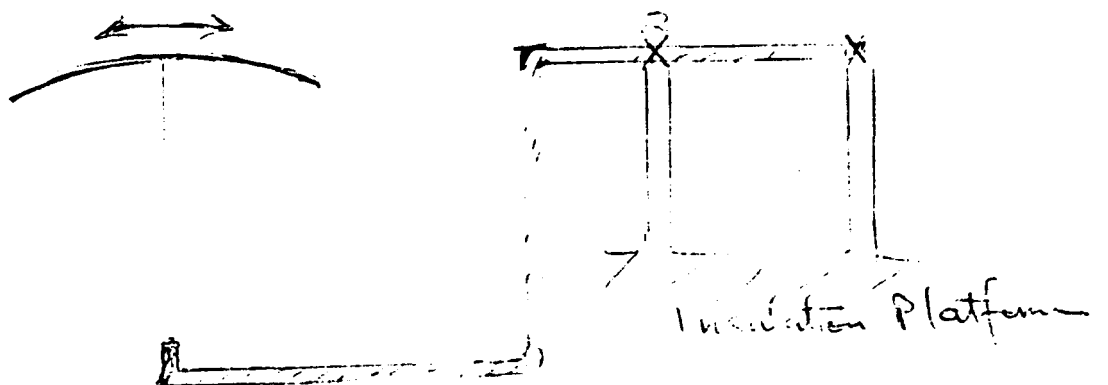
#### 4. Experimental Considerations

The experimental determination of the accommodation coefficient  $\sigma_t$  of the tangential momentum is essentially a force measurement. At the shuttle orbital altitudes of 200-300 Km, the dynamic head  $\rho U^2$  is of the order of 1-10 dynes/cm<sup>2</sup>. Even for a huge test area such as a square meter, the force to be measured is only a few grams weight. Direct force measurements in such an environment may not be as accurate as desired. Moreover, the instrument package for insitu measurements, attached to or otherwise on board of the shuttle is subject to vibrations. Therefore, we are in favor of the following scheme of indirect measurements using a vibrating system that can be effectively "insulated" from shuttle vibrations through frequency modulations. We feel that measurements of amplitude modulations, like decay rates may not be as accurate, nor so easily isolated from the prevailing "noisy" environment.

The vibrating system will be schematically described as follows:

A shaped, "rigid", "convex sheet (a layer or a structure) of test material is supported symmetrically by a "rigid" structure to vibrate in a lateral plane

about a point (or axis) 1 where the normal forces on the sheet surface intersect. We measure the stresses around this point as functions of time (oscillograph to be recorded on tape for further analysis) due to the lateral vibration of the structure carrying the sheet of test material. Past this point, the supporting "shaft" turns a right angle but remaining in the lateral plane



supported by bearings insulated vibrationally but attached to the shuttle. This supporting shaft is to be instrumented at some convenient location 2 to measure the stresses due to the instantaneous net normal forces acting on the test surface. The normal forces acting on the test surface will force the structure to oscillate about 2 with its lateral vibrations. The whole structure should be mounted on a platform, "insulated" vibrationally from the supporting structures attached to the shuttle. We attempt to measure the variations of the tangential and the normal forces on the test surface simultaneously to avoid "mismatching" the oscillatory data for the tangential and normal components in separate vibrating systems. The present gas-surface interaction theory suggests some coupling of the tangential and the normal components through both accommodation coefficients  $\sigma_t$  and  $\sigma_e$  and the surface temperature  $T_w$ , hopefully maintained constant and uniform over the test surface during the experiment. Proper matching of the temporal data of the oscillatory system is essential in the data

reduction.

We suppose that various stress components at each station (1,2) are to be measured electronically such as with the strain gauges, and the electric signals from various gauges over the two stations will be "synchronized" for the present purpose. This synchronization should not be difficult because the oscillatory frequency(ies) in question is likely small, or will be designed to be so.

The assembly should be calibrated and tested in some "High vacuum" environment in laboratory on ground facilities, to fully document the "natural" vibration characteristics of the assembly with gravity compensated in the appropriate frequency range, at least in so far as the "Compound pendulum" representation of the oscillatory system in the "weightless" condition of operation in orbit. We may have to check this while in orbit.

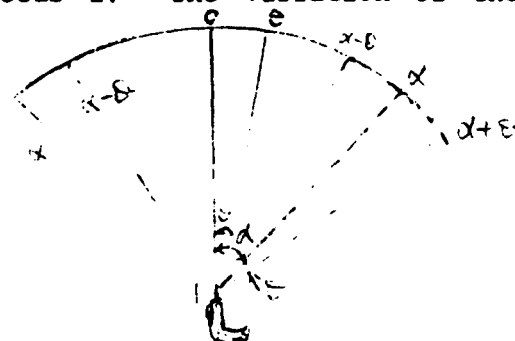
When the instrumented assembly is exposed to the incoming hypersonic stream, the surface is subject to both the tangential and the normal forces. A period of transition of forced oscillation may be necessary to enter itself into an equilibrium vibrating state under the specific forcing function, (i.e. a forced vibration mode). The forcing function is directly related to the ensuing vibration characteristics. We hope that the specific configuration of the vibrating system may separate the lateral and the normal modes. The lateral oscillation about focus 1 is aimed at the exciting forces tangent to the test surface, any residual effects of the normal components will hopefully be minimized. The oscillation about focus 2 is aimed at the normal forces.

If we construct the instrumental package with appropriate rigidity, so that the ensuing vibrations remain small and in the linear range, (i.e. small deflection angle  $\theta$ ), the forcing function will be linear with  $\theta$ , i.e. the resultant exciting moment about focus 1 due to the net tangential forces acting

along the test surface is proportional to  $\theta$ . Within the present formulation of the gas-surface interaction and the hypersonic rarefied aerodynamics theory, this resultant moment of force will be linearly proportional to  $\sigma_t$ , the local accommodation coefficient of the tangential momentum. With the vibrational characteristics of the system fully calibrated and all the relevant constants known, analyses of the stress variations at focus 1 (or comparison with calibration curves under simulated forced oscillation conditions) will permit us to determine  $\sigma_t$  directly.

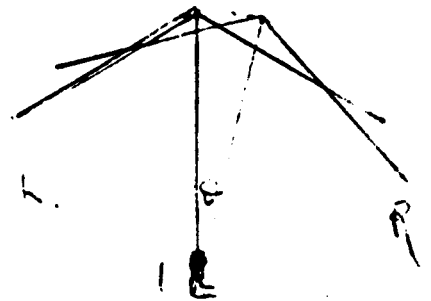
For the vibrations about focus 2 in the transverse plane of the lateral vibration of the test assembly, the shear components of the stresses on the test surface are hopefully minimized or rendered less effective by the geometric configuration, such that the forcing function of the vibration about focus 2 will be excited largely by the variations of the normal forces on the test surface. We hope that the measured stress variations of the shear and the normal forces of excitation may be nearly proportional to the accommodation coefficients  $\sigma_t$  and  $\sigma_e$  of the tangential momentum and energy respectively. Any redundancy in the measurements will provide consistency checks to increase the quality and reliability of the data. If the oscillation at focus 2 is more complex than the presumed simple harmonics, there is no reason why we can not analyze the somewhat more complex situation(s).

It is convenient to use a test surface in the form of a circular arc (cylinder sheet) with its center located at focus 1. The vibration of the surface with an instantaneous displacement  $\theta(t)$  from its equilibrium position simply means the presence of an overhung arc from  $\alpha - \theta$  to  $\alpha + \theta$  beyond the center



symmetric portion of the arc, contributing to net force (and moment) on the surface at the instant. Such an arrangement can be convenient in the analysis of the hypersonic flow field. It also facilitates the visualization how the forcing function acts on the systems as a modulation (decrease) of the restoring moment (i.e. rigidity) of the vibrating system. As such we expect modulations of both the frequency and the amplitude of the oscillation vis a vis those of the natural oscillation calibrated in the laboratory. Indeed such forced oscillations can be simulated in the laboratory prior to orbital measurements to help better designing the experiments and easier reduction of the actual orbital data. The frequency modulation should be essentially linear with the exciting force i.e. with the accommodation coefficient  $\sigma_t$  of the gas surface interaction. The amplitude modulation in the equilibrium oscillatory state will primarily depend on the presence of any inherent damping in the system, which could of course be compensated in the design of the system so as to maintain a neutral natural vibration when not exposed to the external hypersonic stream. Then any additional appreciable amplitude modulation would suggest a mechanism of tangential momentum accommodation somewhat more complex than the linear model.

If the test surface is to be constructed as a pair of plates, symmetrically placed with respect to its equilibrium position. The aerodynamic situation is more complex. It is clear, however, that at sufficiently small  $\theta$  (i.e. less than the swept back angle of the plate) as sketched in the accompanying diagram, the aerodynamic force (moment about 1) on the right plate (R) is larger than that on the left plate (L). As such, it tends to cause frequency modulation of the vibrating system (from its



natural vibrating state). If the angular displacement  $\theta$  is sufficiently large (i.e. larger than the plate swept back) the frictional forces on both plates would tend to destabilize the oscillation. While the vibrating system originally in its natural state need not be destroyed if the system is sufficiently stiff (i.e. large restoring moment), the dynamic behavior of the disturbed system becomes somewhat more complex; and the analysis of the data would be correspondingly more difficult.

The two samples illustrated here are not meant to suggest an optimal choice of test surface configuration, but to illustrate that proper attention to such details can be beneficial if not crucial. The first choice of circular arc is analytically convenient but may not be so structurally, and dynamically there is still the open question of appropriate plane form of a sharp-edged rectangular projection or of some other rounded plan forms to avoid "spurious modes" of vibrations of the test surface. We suppose therefore, a careful laboratory vibration studies of the natural modes of the structure with mounted test surface be conducted and of the oscillatory modes under simulated forcing functions.

In view of the fact that the aerodynamic forces are small and can vary over several orders of magnitude at different altitudes, the vibrating system must possess the appropriate inertia and rigidity to bring about some distinct natural frequency, easily insulated from the inherent vibrations of the shuttle, as the operating frequency. Moreover, they should be chosen such that the small exciting aerodynamic forces will bring about modulations that can be measured easily and accurately. While we can detect frequency modulations to amazing number of significant figures, we are handicapped by the "noisy environment" on board for the insitu experimentation. A careful design of the experimental package cannot be over emphasized. With such attentions to the details, in the

design of the experiment, we believe that meaningful results of such accommodation coefficients  $\sigma_t$  and  $\sigma_e$  can be obtained at orbital altitudes. Our experience with the orbital measurements will be highly helpful in designing further experiments at lower altitudes including the transitional range. We feel that such additional tests are necessary since, in the present theory of gas surface interaction, their independence of external environment and their being a local surface property alone are presumed tacitly without justification, however transparent intuitively it may be.

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## Appendix 6. External Flow Solution

The external flow solution for the SUMS was supposed to be provided by the DSMC computation. It has been under development for some years and reasonable results appeared to have been obtained with suitable choices of computational parameters. The DSMC method will provide specific numerical results but little physical understanding. We hoped that the more carefully computed DSMC results would give distribution functions more nearly self-consistent than the solution due to Bienkowski from which we selected the inlet data for our parametric study. The DSMC external flow solution and the internal flow solution together can be iterated to provide numerical answers to the outflux into SUMS reservoir when the internal flow is choked. Such DSMC computations are tedious and expensive and is slow in coming.

If the external flow solution can be developed according to the beam theory, we would at least have a more consistent approach to the reduction of SUMS data. The external flow problem of rarefied gas flow over the shuttle nose is little less than the problem of rarefied-continuum transition of the flow over a general convex body. The method would be equally applicable to the solution of aerodynamic problems over the lifting and/or maneuverable vehicle in the trans-atmospheric regime. In this context, it is pertinent to recall the popular Newtonian approximation as the limit of  $M_\infty \rightarrow \infty$  of hypersonic continuum flow over a convex body. The Newtonian Approximation is actually based on a free molecular flow both outside and inside a "Shock layer" wrapped around the body. The shock layer is formed by the incident molecules leaving the body surface nearly tangentially after losing all the normal momentum upon impact. The Newtonian Approximation turns out to give a very good estimate of the surface pressure, and

hence the aerodynamic forces on the body in the continuum hypersonic flow regime at modestly large Mach numbers. The modified Newtonian with centrifugal force correction and normalization over the stagnation point gives even better agreement with hypersonic wind tunnel results. This modified Newtonian approximation has been extensively used in engineering estimates of aerodynamic forces in the hypersonic regime. Many attempts to correct the Newtonian approximation within the Navier-Stokes (continuum) framework to extend its applicability to finite, large Mach numbers have not, however, been as successful. The Newtonian approximation should not be perturbed as a continuum but as a transitional flow. The beam method described earlier for SUMS problem is actually a perturbation of the Newtonian approximation for the analysis of the aerodynamic flow in the transitional flow regime.

The Newtonian is free molecular, totally ignoring gaseous intermolecular collisions even in the "shock layer." It emphasizes the interaction of an incident gas molecule and the wall. The model of the gas-wall interaction is such as to have the normal momentum fully accommodated, i.e. lost or transferred in its entirety to the solid wall as if the collision is perfectly "inelastic," ( $\sigma_n = 1$ ), while the tangential momentum is not accommodated at all as if it were in a perfectly "elastic" collision ( $\sigma_t = 0$ ). There is no good reason why the accommodation coefficients for different momentum components cannot be significant different. Indeed  $\sigma_t$  should take some suitable value necessary to remove the reflected molecules to keep the incident molecules from accumulating on the body surface. The reflected molecules tend to form nevertheless, a conspicuous "shock layer" along the convex surface through which the incident molecules have to travel free from inter-molecular collision to impinge on the solid surface within the Newtonian Approximation. The modified Newtonian

introduced the centrifugal correction by claiming that the reflected molecules are moving along the curved surface such that the "shock layer" may coincide with the body surface. The curvilinear motion introduces a centrifugal correction to the surface pressure but the origin of the needed centripetal force was not identified. The centripetal force cannot possibly be provided by the incident molecules, travelling through the "shock layer" without intermolecular collisions. With all the reflected molecules confined to leave along the curved surface, the shock layer is replaced by a thin, dense gas layer likely to intercept the incoming free molecular flow before they encounter the solid wall surface.

Our beam model, introduced earlier for the treatment of the internal flow problem, reconciles the situation in the following manner. The free molecular flow is interpreted to mean that gaseous mean free path is much larger than the characteristic body dimension. Within the space of a body dimension around the surface, the intermolecular collisions between the incident are negligible compared to their collision with the solid surface. When the solid surface is "bare" or "clean", an incident molecule may impact "inelastically" with the wall, give up all its normal momentum. The incident molecule may be trapped or may leave the solid convex surface tangentially with some tangential velocity but cannot escape the surface potential. In other words, the molecular surface potential provides the centripetal force necessary to hold the reflected molecules for them to move along the curved surface.

The molecular population in the surface layer will soon build up to form an absorbed molecular layer of gas over the curved body surface. From then on the incident molecules will collide with the adsorbed gas molecules rather than with the surface. The adsorbed gas layer may thus be set in motion along the curved

body surface. The accumulation of the adsorbed gas molecules will weaken the surface potential such that incident molecules will lead to the emission of adsorbed molecules. The molecules emitted from the adsorbed layer will carry with them certain fraction of the excess momentum and energy of the incident molecules such that  $\sigma_t$  and  $\sigma_e$  may be anywhere between 0 and 1. With sufficient accumulation of adsorbed molecules, an equilibrium state will be reached that on the average, an incident molecule will cause the emission of an adsorbed molecule. The relaxation time for the adsorbed layer to exist and re-established its equilibrium state is much too short to be considered in the flow field. Thus the emitted molecule may as well be considered as the "reflected molecules" especially when the incident and the adsorbed molecules are of the same kind. For aerodynamic purposes, the body surface may then be considered as always covered by an equilibrium adsorbed gas layer. The conservation relations of such an equilibrium adsorbed surface layer will limit the range of variations of the accommodation coefficients for the prevailing surface conditions.

The assumption of free molecular flow outside the equilibrium adsorbed gas layer of a few molecules thick over a convex solid surface and the choice of  $\sigma_t = 1$  will reduce our beam model to the Modified Newtonian approximation. The free molecular outer flow makes it unnecessary to choose  $\sigma_e$  since the collisions between the diffusely emitted thermal beam from the adsorbed layer with the incident molecules are neglected. In this sense, the internal flow solution presented in the previous sections based on free molecular gas flow with exclusive gas-wall interaction may be considered as an "Extended Newtonian" solution for the internal flow configuration. For the external flow problem, the diffused thermal beam of molecules will collide with some incident molecule upon penetrating the incoming beam for a few mean free paths. The collisions between

the diffused molecules of the emitted beam with those nearly mono-energetic molecules will collide with some incident molecule of the incident beam will randomize both to become the diffused constituent of the gas "mixtures" approaching the body surface. Thus the mole fraction  $\beta$  of the incident beam will decrease gradually from unity beginning a few mean free paths away from the body surface to achieve some value  $\beta_s < 1$  upon reaching the solid surface. It then drops "discontinuously" to zero across the adsorbed gas layer on the solid surface. The modified Newtonian is the idealized limiting case with  $\beta = 1$  extending all the way to the adsorbed gas and with  $\beta$  dropping to zero discontinuously from unity, upon reaching the surface. Such is clearly the case when  $K_N$  is sufficiently large.

When the gaseous mean free path of the Knudson number  $K_N$  decreases from large values toward  $O(1)$ ,  $\beta_s$  will drop from near unity toward zero. At some value of the Knudson number of  $O(1)$ ,  $\beta_s$  will vanish on the solid surface with a finite nonzero slope (i.e.  $\beta_s = 0$  ( $\frac{\partial \beta}{\partial n})_s \neq 0$ ). With further drop of the Knudson number, there will no longer be any discontinuous jump of  $\beta$  across the adsorbed gas layer. Continuum flow conditions (possible with slip) has been reached locally, next to the solid surface; and transition from the rarefied to continuum flow states takes place across some "shock", extended by detached from the vehicle surface. These events are sketched in the accompanying figure how the flow transition will take place according to our beam method.

The special "free molecular flow" limit with  $\sigma_n = 0$  and  $\sigma_t = 1$  is identified as the Modified Newtonian approximation. Within our model of gas-wall interaction, we see no good reasons why  $\sigma_n$  and  $\sigma_t$  should not take other values between 0 and 1 while the external flow is free molecular. Therefore our beam model would suggest that at orbital altitudes suitable choices of the values of  $\sigma_e$ ,  $\sigma_t$  will provide better estimate of the aerodynamic forces etc experienced by satellites in orbit. When the  $K_N$  decreases at lower orbital altitudes the essential correction over the modified Newtonian lies in the presence of gaseous collisions that reduce the mole fraction  $\beta$  of the incoming gas from unity prior to their arrival on to the surface (or the adsorbed gas layer). The molecular distribution function remains highly nonequilibrium with  $\beta \neq 0$ , since the incoming nearly mono-energetic molecular beam simply has been little diffused by the molecules from the surface. Therefore corrections to Newtonian should be attempted within the rarefied rather than the continuum framework.

The DSMC method attempts to describe the evolution of the distribution function of the gas molecules coming onto the surface by the simulated collisions among the Monte Carlo particles (MCP). The collisions among such MCP's is generally taken to be the same as molecular collisions, relying on the Central Limit theorem to use repeated sampling among the much smaller ensemble to generate an adequate approximation of the molecular distributions function. When the central limit theorem has to be abandoned for the hypersonic nonequilibrium flows, we would have to consider such MCP as having some sort of internal equilibrium. These micro ensembles of Monte Carlo particles will undergo randomizing collisions according to some collision model of collective systems (Not individual molecules). The DSMC computations can track such randomizing collisions provided that some collision model of such collective micro systems

can be developed. We have little guidance to do so.

The present beam method identifies the uncollided incident molecules as beam 1, which retains its undisturbed mean flow property but decreases in its relative population  $\beta$  due to randomizing collisions with the a diffused beam, beam 2. This diffused beam 2 is presumed to possess its own equilibrium distribution with mean properties evolving according to the global conservation principles. These global conservation relations can be obtained as some moment approximations of the Boltzmann equation with the composite distribution function, integrated over the appropriate velocity spaces. We suppose that such global invariants are more directly related to the physical phenomena of interest and may yield better and internally more consistent approximations to the solutions of practical aerodynamic problems, including the SUMS internal and external flow problems. The mass flux through SUMS Inlet is presumably small and negligible in the external flow solution for the mean flow properties over SUMS Inlet. If "choking" of the internal flow should indeed take place in the reduction of SUMS data, and if the external flow solution is locally not so stable, both the internal and the external flow solutions may have to be iteratively corrected. The matching of the external and the internal flow solutions can be somewhat complex but surely can be consistently developed based on the same beam method.

To formulate the external flow problem for solution, we consider an incoming nearly mono-energetic hypersonic beam of molecules, beam 1, and a diffused beam of molecules, beam 2, emitted (or reflected) from the adsorbed molecular layer on the solid surface. The inter-beam molecular collisions, convert beam 1 molecules into beam 2, such that the mole fraction  $\beta$  of the beam 1 molecules decreases toward equilibrium molecular distributions around their respective mean properties. The mean properties of beam 1 remains unchanged from the values of

the undisturbed atmosphere far away from the vehicle. The mean properties of beam 2 changes toward the surface upon increased conversion of beam 1 molecules into beam 2. The solution of the external flow problem involves the determination of the evolution of beam 2 mean properties and the mole fraction  $\beta$ . For convenience, we define a mean gas, as is described in Appendix 1, which is a mixture of two gases of the same chemical nature but at different thermodynamic and kinetic states. Each constituent gas possesses its own molecular distribution function  $f_1$  and  $f_2$  about its own mean values.

We express the molecular distribution function of the mean gas as

$$f = \beta f_1 + (1-\beta) f_2 \quad (1)$$

where  $f(\beta, x_j; c_i; t)$  and  $\beta(x_j, t)$ .

Substitute this into the Boltzmann equation (consider velocity space only)

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial c_i} = \int_c \quad (2)$$

which expresses the conservation of molecules in the velocity space. The right hand side is the collision integral that accounts for the net changes of the molecular population in a given element of velocity space by the collisions among all the molecules. Since we are interested only in the evolution of the average properties of such a system, we multiply this Boltzmann equation by  $m$ ,  $mu_i$  and  $me$  (the molecular mass, momentum and energy) and integrate over the velocity space of beam 1 and beam 2 respectively to generate two sets of evolution equations for the mean properties of beam 1 and beam 2 respectively, a total of 10 partial differential equations, 5 for each beam.

With the mean properties of beam 1 remaining constant, the system for beam 1 degenerates into a single equations describing the evolution of  $\beta$  due to interbeam collisions, visualized as beam 1 being scattered by a diffused beam of molecules issued from the vehicle surface. We integrate this differential



relation approximately to obtain

$$\beta = \frac{1}{\rho} \exp \left[ -\frac{c}{K_N} \left( 1 - \frac{1}{\rho} \right) \right] \quad (3)$$

which gives  $\beta = 1$  when  $\rho = 1$  far away from the vehicle surface. The fraction of undisturbed incident molecules arriving at the surface is  $\exp \left[ -\frac{c}{K_N} \left( 1 - \frac{1}{\rho_s} \right) \right]$

that depends very strongly on the  $K_N$ . With surface density  $\rho_s > 10$  and  $c \sim 1$ , transitional flow characteristics will manifest when  $K_N \sim 1$ , i.e. around 120 Km. altitude. The parameter  $c$  largely represents the scattering collision cross section of the molecules.

We transform the mean flow equations of beam 2 to those of the mixture by letting  $(1-\beta)\rho_2 = \rho - \beta\rho_1$ , etc. We obtain

$$\begin{aligned} \frac{\partial(\rho)}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} &= 0 \\ \frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} &= 0 \\ \frac{\partial(\rho e)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j e) + \frac{\partial q_i}{\partial x_i} - D &= 0 \end{aligned} \quad (4)$$

where  $\tau_{ij}$  represents the  $i$ th component of the global stress acting on the  $j$ th surface,  $q_i$  the heat transfer vector across the  $i$ th surface, and  $D$  the dissipation. This set of mean flow equations for the mixture stands in the same form as the Navier-Stokes equations system for the continuum gas flows, except that  $\tau_{ij}$  and  $q_i$  are no longer given by the continuum expressions in terms of the local mean flow gradients.  $\tau_{ij}$  consists for example of two parts. One part represents the net momentum transport across a surface due to the random components superposed on the mean motion of beam 2. The other part arises from the non-equilibrium state that beam 1 and beam 2 molecules possess significantly different properties  $\sim \beta (1-\beta)(u_1 - u_2)^2$  for example. If we wish to solve for the mean flows from equations system (4), we first have to decide on the constitutive relations defining the  $\tau_{ij}$ ,  $q_i$  and  $D$  in terms of the mean properties of both

beams and the mole fraction  $\beta$ . We may know enough of basic physics to do so; but the resulting model constitutive relations are necessarily too complicated and with too many adjustable constants. It is possible but judged not really meaningful within the context of SUMS program to attempt direct solution of the partial differential equations system such as the kinetic equations solved in the Soviet Literature.

In so far as our interest lies primarily on flow properties along the vehicle surface, and for the present project the flow properties over SUMS inlet order, we shall try to solve for only the surface properties through some integrated form of equations system (4), under suitable assumptions to facilitate the integration. The contributions from the stress  $\tau_{ij}$  and heat transfer  $q_i$  in the integrated equation system will be limited to the surface stress and heat transfer rate "on the solid surface", which can be formulated for an equilibrium adsorbed molecular layer covering the vehicle surface through the accommodation coefficients  $\sigma_t$  and  $\sigma_e$ . To simplify the geometry we shall we adopt the tangent cone approximation with the conical element taken as the meridian section of the shuttle passing through SUMS Inlet. The external flow problem is thus reduced to the solution of the hypersonic rarefied gas flow over an axisymmetric convex body section defined as  $r_s(z_s)$ . We take as the conical axis, coinciding with the incoming flow,  $r$  as the radius in the transversal plane and the subscripts designates the surface value with  $r_s(z_s)$  describing the meridian curve of the convex axisymmetric body.

We write system (4) in the cylindrical coordinates  $r, \theta, z$  with  $\frac{\partial}{\partial \theta} = 0$ .

Assume exponential decay of various mean properties from the surface  $z_s$  with logarithmic decay rates  $\alpha_u, \alpha_v, \alpha_p, \alpha_e$ , for radial and axial velocity components,

density and internal energy respectively. They assume their surface value at  $z = z_s$  and the values of 0, -1, 1 and 1 at infinity  $z \rightarrow \infty$ . These  $\alpha$ 's are in principle function of  $r$  that assume some finite value on the axis  $r = 0$ , and become very large where free molecular conditions prevail as the solid surface terminates in the radial direction. We shall take  $\alpha$ 's as locally constants in deriving these equations for numerical integration of the resulting equations system in the  $r$  direction in which the values of  $\alpha$  will be taken differently in different segments according to some integrated criteria. The differential equations system for  $u_s$  vs  $\rho_s$   $e_s$  with  $\beta_s$  given by equation (3) in terms of  $\rho_s$  are very complicated algebraically even with  $\alpha$ 's independent of  $r$ . We attempt to integrate numerically from a given set of initial data of  $u_s$   $v_s$   $\rho_s$   $e_s$  at  $r = 0$  outwards through successive rings as  $r$  increases until  $r = 1$  where the solid surface terminates. The values of  $\alpha$ 's are to be chosen in successive rings such that the global conservation of mass, momentum and energy are satisfied for the enclosed cylindrical space. The surface pressure, wall friction and heat transfer and the surface flow properties of the mean gas with mole fraction  $\beta$  are all determined successively at all  $r$  for each time step. We hope to have the system evolve until some quasi-steady state is approached at some large time. We are developing the details of such a numerical solution of the external flow problems. This is not trivial in view of the "sonic singularity" present in the system at some unknown location. We believe it to be manageable with reasonable amount of effort.

## APPENDIX 7

### HYPersonic PROPULSION

by

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#### ABSTRACT

The recent revival of hypersonics is much related to the development of SCRAMJET as the latest airbreathing power plants for aero-space applications. We shall review first the whys and hows of the concept of supersonic combustion for hypersonic propulsion without indulging in the design and performance details. We shall identify the problem areas, describe the current research and development efforts and explore their implications. The operating boundary of SCRAMJET is reasonably well defined. It is suitable for selected missions. We shall then explore briefly some airbreathing alternative that may go beyond SCRAMJETS.

## 1. INTRODUCTION

Hypersonic Flow is meant to be the flow of air (or other gas mixtures) over a body or surface at a speed  $U$ , much larger than the speed of sound  $C$  in the gas. The speed of sound  $C$  in earth's atmosphere is remarkably constant  $\sim 0.3 \pm 0.05$  km./sec or  $1 \times 10^3$  f.p.s. at almost all altitudes while its density and pressure drop very steeply, roughly by a factor of  $10^{-3}$  for every 50 Km. rise in altitudes. Hypersonic speeds in earth's atmosphere are often taken to mean a couple of Km/sec and up with flow Mach numbers  $M = U/C > 5$  considered as  $> > 1$ . For earth orbital missions flow Mach numbers are often as large as 20-30. A propulsion device (or an engine, power plant) is to generate thrust to overcome the aerodynamic drag on the vehicle and with remaining net thrust to overcome the vehicle inertia in gaining kinetic energy (or speed) and altitudes (against earth's gravity) when needed.

Generally speaking aerodynamic drag  $D$  and aerodynamic heating increases with Mach numbers as  $M^2$  and  $M^3$  respectively for a hypersonic flight at a given altitude i.e. with a nearly constant atmospheric density  $\rho_\infty$ . Thus hypersonic flight implies a very high drag and heat load except when the local undisturbed static atmospheric density  $\rho_\infty$  or pressure  $p_\infty$  is much less than those at ground or sea levels. High drag means high expense of propulsive power for maintaining level flights; and high heat flux means serious complications of heat shield for surviving the adverse thermal environment. Sustained hypersonic flights (or cruise) are therefore meant to be at high altitudes. Thus cruise at  $M \sim 5$  to 6 may be considered at altitudes 30 ~ 40 km. above S. L. where  $\rho_\infty/\rho_{SL} > 10^{-3}$  with reasonable drag and heat load. Mach 15 to 20 flights at such altitudes would encounter excessive drag and adverse thermal environment comparable to those of reentering ballistic nose cones. Sustained hypersonic flights at such high Mach

numbers therefore appear to be sensible only at altitudes 80 Km and above with  $\rho_\infty/\rho_{S.L.} > 10^{-6}$ . Even then, the heat load and the drag on such vehicles can be significant. Cruise at satellite altitudes of  $\geq 300$  Km, where the air density is so low as to be considered as "vacuum", requires little thrust or thrust power of the propulsive devices. The selection of power plants for a hypersonic vehicle is therefore not dictated by the economics of operation at cruise as is for conventional airplanes but by the requirement(s) of significant maneuver such as orbital transfer or the lift off from ground into the desired trajectory. For the latter, we have to operate throughout the entire altitude range from the conventional continuum aerodynamic regime to the rarefied gas regime near vacuum. Such drastic changes of the operating environments of hypersonic vehicles call for different power plants in different regimes and for different vehicle missions.

The overall requirement of any hypersonic propulsion system is to generate net thrust that transfers energy to the payload so that the payload can achieve the appropriate velocity in the desired orbit. The level of the net thrust provided by a propulsive device(s) determines the time required to accomplish a mission. Since the kinetic energy of an orbiting vehicle is much larger than its potential energy in Earth gravity field, the minimal global energy requirement of a hypersonic propulsion system is to have its time integral

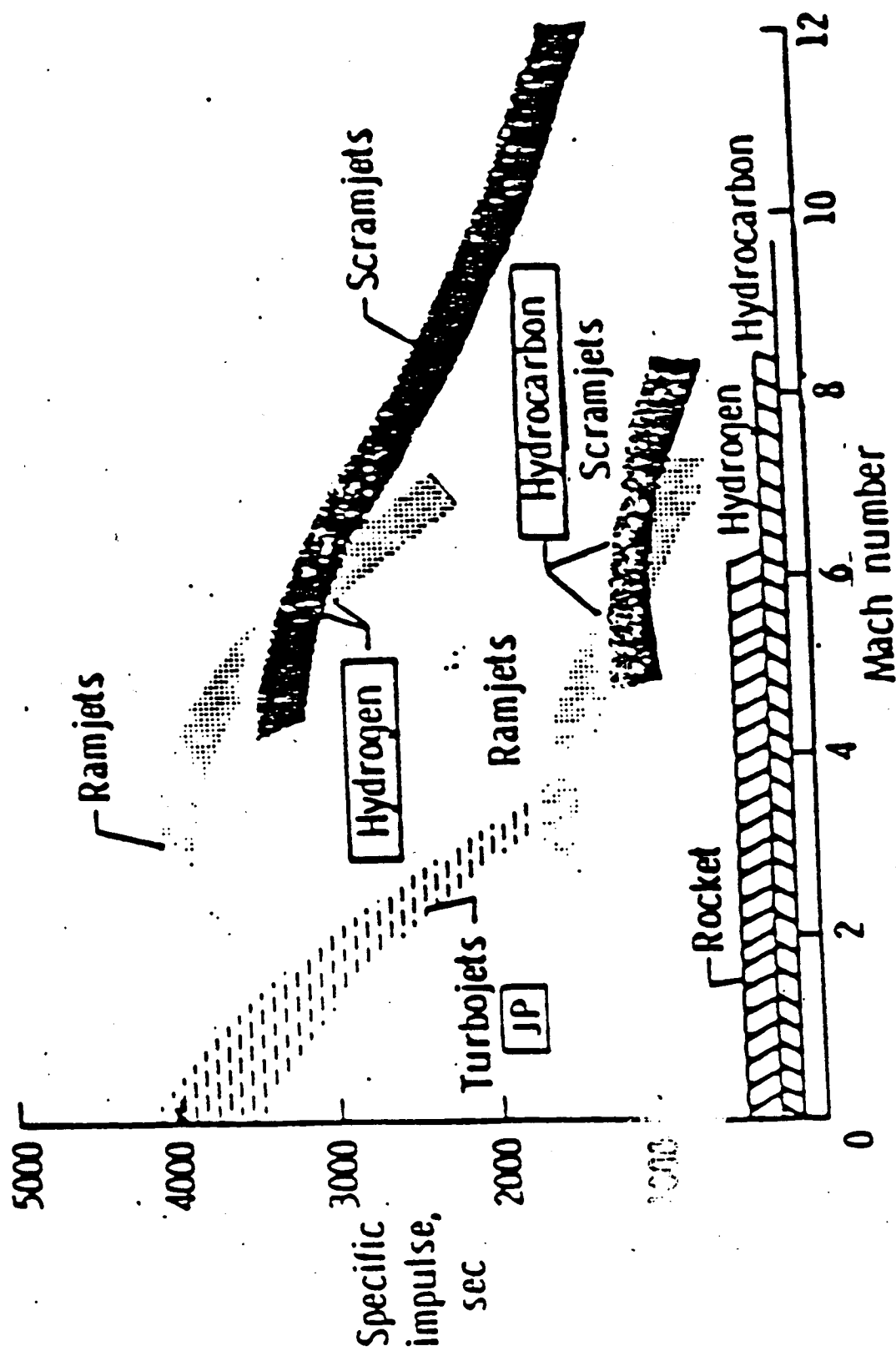
of the net thrust power  $\int_0^t (T-D) u \, dt$  exceeding the kinetic energy of

the orbiting payload. The vehicle velocity  $u(t)$  depends on the integral of the net thrust  $T-D$ ; and the vehicle trajectory including its altitude depends on the integral of  $u(t)$ . The dependence of  $T-D$  on altitudes is critical in the choice of the appropriate propulsive device(s). Where air is abundant, airbreathing propulsion devices are preferred since they derive more than 80-90% of the

propulsion medium from air "free". Where ambient air is not available all the propulsive medium must be provided as propellant to be carried on board of the vehicle as is in rockets. There are various (non-exotic) propulsion alternatives inbetween as illustrated in Fig. 1, and many more as combinations of different alternatives. The fuel specific impulse  $I_{sp} \sim (T/m_p)(m_p/m_f) \sim (m_p/m_f)u_e/g$  as the key performance parameter of each type of power plant varies as a functions of the operating Mach number at altitudes appropriate for the power plant. A hypersonic mission can be carried out by varieties of mixes of such alternatives with quite different thrust programs  $T(H)$  or  $T(t)$ . The specific choice of the type of propulsion device determines to a large extent the thrust programs, the trajectories and the economics of accomplishing a specific mission.

In the early hypersonic era of 1950's the primary missions were to put payloads into low earth orbits or suitable ballistic trajectories. For such missions, we have to lift the payload from its base, boost it to hypersonic speeds, let it coast powerlessly toward the orbit and finally inject it into the required trajectory. All these can be accomplished through multi-stage rocket motors. Multi-staging is needed because of the limited specific impulse of rocket propellants, and provides us the opportunity to discard the spent motor(s) from being carried on board to higher velocities. Rockets are essentially constant thrust devices, largely independent of the ambient atmospheric environment so that thrust programming is greatly facilitated. During the lift off and the boost phase in the lower atmosphere, airbreathing power plants with free oxygen supply from the ambient air appear much more attractive than booster rockets that have to carry the oxidizer along with the fuels. Even the inert nitrogen in the atmosphere can be utilized to augment thrust through larger mass flux of the propulsive medium. Thus, a hybrid propulsion system with upper

# PROPULSION ALTERNATIVES





rocket stages piggy-backed on a conventional airplane was considered as early as 1950's. The complexities of such a hybrid system and the need to develop the giant airplane first stage apparently outweighed the advantages. Thus, hypersonic vehicles have always been launched with multi-stage rockets, using liquid and/or solid propellants. The successful development of the ever more powerful rocket boosters has established the multi-stage rockets as the first generation hypersonic propulsion system. The economy of launching hypersonic payloads was pursued through the development of the space shuttles with reusable heat shield and refurbishable rocket boosters.

Aerothermodynamic analysis and computation of the reactive flow of high temperature gases played an important role in the design of the heat shield for the survival of both the ballistic nose cones and shuttles during reentry through the low dense atmosphere. It has also helped in improving the design of rocket combustion chambers and nozzles. The increasing power and availability of supercomputers naturally enhances our expectations that airbreathing power plants can be made to operate at higher altitudes. Conventional jet engines with separate diffuser-compressor, combustor, and turbine-jet nozzles can serve well above 15 km altitudes and push the assembly to moderate supersonic Mach numbers. The ram pressure recovery of the free stream will then be sufficiently high to provide the pressure ratio needed for nozzle expansions in generating adequate thrust. The turbine-compressor assembly can be bypassed or removed. We have then the conventional ramjet power plant in which the inlet supersonic stream is diffused to some adequate high pressures and low subsonic speeds without compressor power input. Fuel is injected and burned there into hot gaseous combustion products for expansion directly through nozzle to produce thrust. The ramjet is thus little more than a flow reactor, with a high temperature reaction

zone attached to the "injectors" and/or "flame holders" to secure a "complete" release of heat from the fuel-air mixture within the limited space of the combustor.

At higher flight Mach numbers (5-8), the ram pressure ratio (even with normal shock) becomes unnecessarily high for nozzle expansion; while the temperature of the compressed air approaches and eventually exceeds the flame temperature of the fuel-air mixture. The "combustion products" will then remain as various dissociated species. They will release the heat of combustion only upon recombination when expanded to lower temperature and pressure. Such heat addition at lower pressure is less efficient for thrust generation. Thus such subsonic combustion ram jet devices are useful only for vehicles flying at  $M < 8$  in Earth Atmosphere. The air static temperature accompanying the ram pressure recovery to smaller Mach numbers  $M$  is roughly  $T_{\infty}(1 + \frac{\gamma-1}{2} M_{\infty}^2) / (1 + \frac{\gamma-1}{2} M^2)$ . With the static temperature  $T_{\infty}$  of earth atmosphere  $> 300^{\circ}$  K despite orders of magnitude reduction of its density and pressure at higher altitudes, the temperature of the stagnant air increases rapidly with the flight Mach number  $M_{\infty}$ . To limit the air temperature entering the combustion zone for prompt heat addition we can limit the diffusion of the incoming hypersonic stream to some reasonable supersonic (rather than the low subsonic) state. Here arises the concept of Supersonic Combustion Ram Jet, Acronym SCRAMJET, to extend significantly the "Airbreathing Corridor" (Fig. 2) in Earth atmosphere.

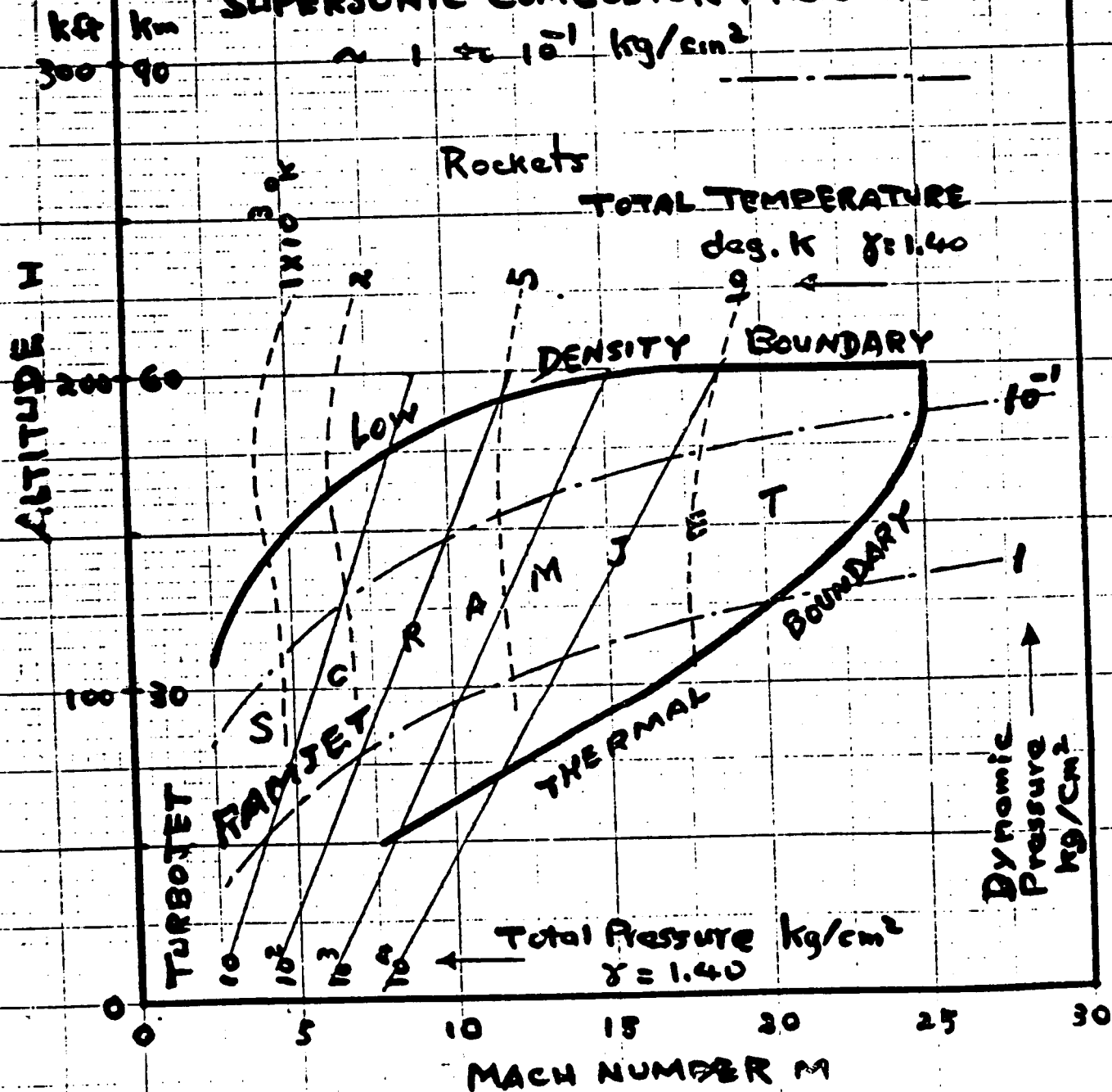
The following questions naturally arise:

1. Can we diffuse a hypersonic stream through a diffuser under varying operating conditions to some stable low supersonic stream without shock transition to low subsonic flows?

# AIR BREATHING CORRIDOR SCRAMJET OPERATING BOUNDARY

SUPERSONIC COMBUSTOR PRESSURE

$$\sim 1 \text{ to } 10^1 \text{ kg/cm}^2$$



ORIGINAL PAGE IS  
OF POOR QUALITY

2. Can we inject and burn the fuel in a supersonic stream without causing subsonic out flow of combustion products from the " supersonic combustor"?
3. What will be the operating range (the airbreathing corridor) of the SCRAMJET and the improvement in the economy of boosting specific payloads into hypersonic trajectories in different missions?

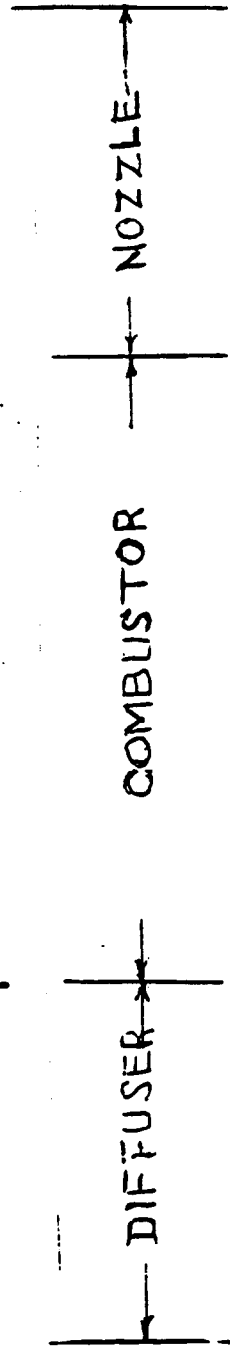
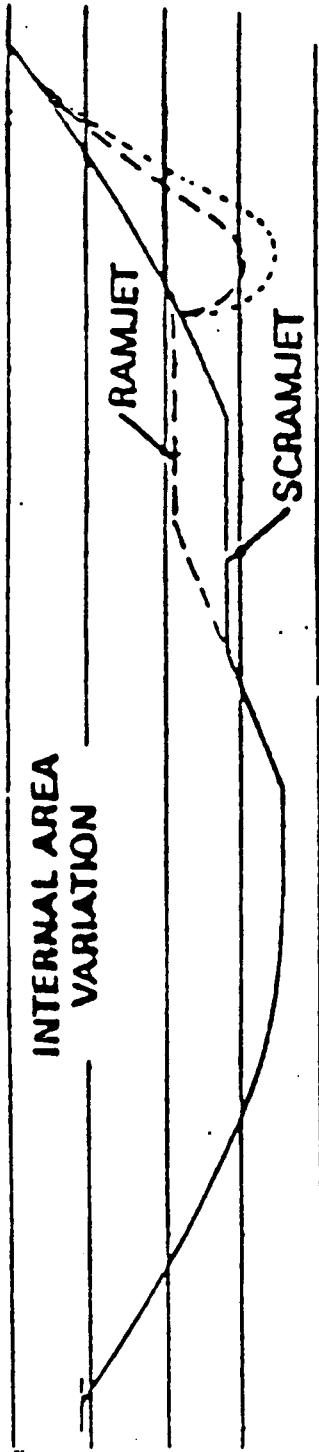
Many experiments have been performed since early 1960. Research and development activities have intensified greatly since 1970's after successful launches of the space shuttles. Optimism now prevails that SCRAMJET is destined to be the propulsion system for the much publicized Aero-Space Plane for hypersonic flights from Washington D.C. to Tokyo. Such a hypersonic vehicle with a SCRAMJET power plant will surely have an altitude ceiling, a cruising speed and an operating envelope way beyond those of the present day airplanes.

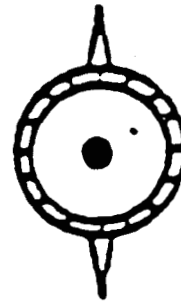
The SCRAMJET is not the answer to all aerospace missions, but can be a common element of the airbreathing part of a hypersonic propulsion system. The SCRAMJET is a focus of current U.S. aerospace research and development. Many preliminary design considerations with extensive literatures are presented in a status report<sup>(1)</sup> at the first Joint Europe - U.S. short course on hypersonics in 1987. Aerothermodynamic computations played a central role in such preliminary analyses<sup>(2)</sup>. We shall not repeat them here. We shall consider only some important features in preparation for further discussion of the various technical and scientific aspects of SCRAMJET.

## 2. SCRAMJET

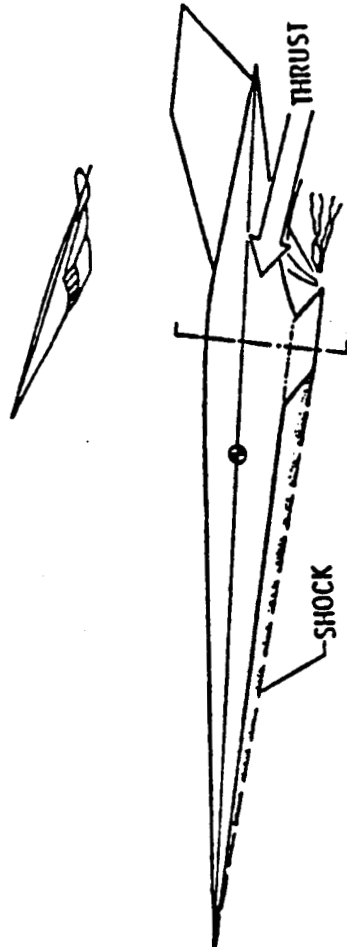
We consider a hypersonic vehicle to take off from near sea level with a conventional jet engine and then accelerate under a subsonic ramjet to some supersonic Mach numbers like 3-4 at altitudes of  $\sim 25$  Km. The vehicle is to be accelerated further to Mach 5-6 for cruise at the prevailing altitude or potentially to Mach 20  $\sim 25$  for entering into earth orbits along selected trajectories with minimal additional rocket power. It may reenter and land horizontally on conventional runways and to take off again after refueling.

The SCRAMJET consists of three basic elements: the supersonic diffuser, the supersonic combustion chamber, and the jet nozzle, much the same as the standard ramjet. The internal area distribution along their lengths are illustrated in Fig. 3 using the same diffuser. The only notable difference is the absence of a sonic throat in the SCRAMJET. The purely diverging nozzle of SCRAMJET appears to be a natural extension of the combustion chamber. The absence of the sonic throat does help to reduce heat transfer problems, although not the major reason why we like to have supersonic combustion for a ramjet. The supersonic diffuser takes in air at low density, say  $\rho_\infty/\rho_{S.L.} \geq 10^{-3}$  around 30-50 Km altitude, and brings it to the entrance to the combustion chamber at some sub-atmospheric density ( $\rho/\rho_{S.L.} < 1$ ). The large compression ratio means a very large ratio of the total Air Inlet area to the area of the combustion chamber inlet. We soon find that the inlet area of the supersonic diffuser will be comparable to or larger than the gross section area of the entire vehicle. Likewise, we find a very large nozzle area to expand the hot gas to the rear. These are important considerations of the air frame design of the vehicle. The hypersonic vehicle will assume naturally a shape with a diffuser in the front and a nozzle in the rear, and with plenty of space inbetween for crews, fuels and payloads in the





Accelerator  
(Flying Engine)



SCHEMATIC OF  
ENGINE CROSS SECTION

"neck" region over and/or around the combustion chamber. Hence the vehicle frame is globally the same as the engine frame, integrated in the very early stage of the design process. This extensive airframe-engine integration provides indeed many advantages. An important consideration is to use the heat flux from the diffuser and the nozzle wall to heat up the fuel (most likely liquid hydrogen in cryogenic storage) before it is injected into the combustion chamber. It also permits sophisticated aerodynamic controls of the air flows in the diffuser and the nozzle to avoid the undesirable shock waves, separations etc for more efficient diffusion and expansion.

The global geometry varies significantly as is illustrated in Fig. 4, much depending on the specific mission. The configuration of an accelerator to deliver large net thrust may be an axisymmetric vehicle with exterior combustion chamber and a tiny wing, i.e. (the flying engine). The cruise configuration of a hypersonic vehicle such as the long range transport may need a significantly larger wing if the cruise altitude is low or the lift for maneuver is significant. The location of the wing relative to the engine and its design may be dictated by aerodynamic considerations that can be much different at different cruise altitudes and Mach numbers. Such three dimensional details are not important for preliminary considerations. We shall ignore the local azimuthal variation of the vehicle configuration, and consider as illustrated in Fig. 3 a section along the plane of symmetry or through the axis of a local tangent cone approximation. We shall also presume that our experience with continuum aerodynamics should apply in anticipation that SCRAMJET is not to operate above 60 Km. Then when the configuration of the diffusion ramp is fixed, an inviscid analysis (or computation) of the two dimensional supersonic diffusing flow will give the shock emanating from the tip of the diffuser and the air mass flux into



the engine cowl or combustor inlet. Since we like to catch as much free stream air for combustion purposes the diffuser ramp should be designed to have the diffuser shock not missing the cowl lip. At the high Mach numbers, the diffuser ramp will be long compared with the local radius. The large compression ratio ( $\rho/\rho_\infty$ ) implies that the clearance of the engine cowl from the diffuser ramp is a small fraction of the local radius. Therefore, the growth of the viscous boundary layer on the diffuser ramp surface will be significant in comparison with the small thickness of the supersonically diffusing shock layer over the ramp. It is imperative to estimate the displacement effect(s) of the viscous layer on the configuration of the diffuser, the shock and the air mass flux through the engine cowl into the combustor. The interaction of the viscous boundary layer on the ramp surface with the supersonic diffusing stream under the shock can be computed even for a large compression ratio and in three space dimensions provided that the boundary layer does not separate.

Under the prevailing adverse pressure gradient the boundary layer is susceptible to separation and cross flows, causing secondary shocks, flow transition to turbulence, unstable operations of the supersonic diffuser, and leading potentially to subsonic diffusing flows. We can prevent this with adequate boundary layer control through some programmed removal of the slow and hot air in the proximity of the ramp surface. Such boundary layer control can be integrated with the heating devices needed to heat the fuel before being injected into the combustion chamber. The bled air may be introduced back into the expanding nozzle gas further downstream to augment the propulsive mass flux. Such a programmable control system is complex and need extensive engineering developments; but there is little doubt that such can be accomplished at Mach numbers 5 or 6, in view of our successes at lower supersonic Mach numbers<sup>(3)</sup>.

The supersonic diffuser does need considerable development, but it is not likely a critical component in the SCRAMJET program.

The supersonic stream is heated to higher temperatures through fuel-air reactions in the combustion chamber. The gaseous combustion products are to be expanded through the nozzle to generate thrust, which hopefully will be more than what is needed to balance the overall drag caused by the high pressure on the diffuser ramp. This is possible because of the significantly lower Mach numbers of the expanding hot gas. Limited by the frontal area, the nozzle is likely under-expanded so that the expansion waves from the cowl lip on the rear should be prevented from striking onto nozzle thrust surface. A good part of the nozzle on the side of the cowl can thus be removed. The free expansion of the hot combustor gas into the ambient atmosphere away from the vehicle is also convenient in providing lift. Thus lift will be derived from the transverse component of pressure forces on both the diffuser ramp and the nozzle thrust surface. The aerothermodynamic computations for the expansion of the hot combustor gas can provide the analytic basis for improving the design of the nozzle contour whether the expanding gas is in equilibrium or not. There is little reason that the thrust nozzle may be a critical component in the SCRAMJET program.

The "supersonic combustor" remains as the focus of current research and development. The combustion chamber of the SCRAMJET is to operate at sub-atmospheric pressures i.e.  $< 1$  kilogram per  $\text{cm}^2$  and at altitudes around 40 Km. This choice largely reflects our familiarity of the fuel-air combustion under such a thermodynamic environment ( $p$ ,  $\rho$  and  $T$ ) and our awareness of the very high compression ratio required of the diffuser and of the inflammability limit of fuel-air mixtures at low pressures. The fuel is preferable hydrogen rather than

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hydrocarbons for the higher specific impulse. The reaction kinetics and the global combustion phenomena of  $H_2$  in  $O_2$  are also better understood. We have much more experience, however, in developing efficient combustors for hydrocarbons in conventional jet engines to achieve almost "complete combustion" in a relatively small volume. The strategy employed in these combustors of conventional jet engines is to slow down the air flow so as to increase the residence time of fuel and air in the combustor for them to mix thoroughly and to burn completely. We even go to the extreme by employing buffer barriers to force the air and/or mixtures to follow some highly contorted paths with flow reversals in the combustors. We employ flame holders to "anchor" the flames at locations where combustion can proceed favorably. Such devices create pressure drops, which are tolerated as necessary and compensated for by compressing the inlet air to higher pressure. Now for supersonic combustion, we do not want to slow the air-fuel mixture down to such low speeds, too hot to receive any further heat from chemical reactions. How are we going to secure a reasonably complete combustion within a tolerable combustor volume?

At around sea level atmospheric pressures, the reaction (or combustion) time of premixed hydrocarbons and air is  $\sim 10^{-3}$  sec., while that of Hydrogen and air is  $\sim 10^{-6}$  sec. At supersonic velocities, such reaction times correspond to reactions zones of meters or centimeters thick respectively. It becomes clear that hydrogen has to be chosen as the fuel for SCRAMJET and correspondingly fast and complete mixing of hydrogen and air must be accomplished. Indeed, complete mixing at  $10^{-3}$  sec levels might still appear too slow. The combustion of gaseous hydrogen in air as a heterogeneous mixture is surely "Diffusion or Mixing Controlled"; and the reaction front in the premixed packet of  $H_2$ -air gas is likely a classical diffusion flame. In other words, the major concern of

combustor design remains the same i.e. to bring about fast and complete mixing of hydrogen gas and air, but now flowing at supersonic speeds which we do not like to have it slow down. We shall discuss this in greater detail in the next section.

As is illustrated in Fig. 2, a SCRAMJET to operate at altitudes say around 50 Km and  $M \sim 15$  will have a combustion chamber pressure of about  $10^{-1}$  atmosphere, despite the large compression through the supersonic diffuser. This is because of the rapid exponential fall of atmospheric density which at  $\sim 50$  Km may be  $\rho/\rho_{S.L.} \sim 10^{-3}$ . Even a compression ratio of  $10^2$  could only bring the air density back to  $10^{-1}$ . At such sub-atmospheric conditions, the reaction time of the premixed  $H_2$ -air will increase significantly if at all ignitable. At still higher altitudes, there could be essential changes in the kinetics of reaction and there could be "flame out". Thus, even if we could achieve instant mixing and the ideal condition of premixed stoichiometric mixture, there will be serious doubts if a SCRAMJET designed for the lower altitudes might remain operable at much higher altitudes. This is the basic reason for the presence of an upper operational boundary of the SCRAMJET as is depicted in Fig. 2. SCRAMJET is clearly a useful airbreathing hypersonic power plant to bring a vehicle from 30 to 50 Km altitude, and from Mach number 5 to Mach 10. SCRAMJET would also serve as the ideal airbreathing power plant for a Mach 5-6 hypersonic cruiser at  $\sim 40$  Km altitude with some reasonable capacity to maneuver.

### 3. Supersonic Combustor

In view of our discussion of the supersonic diffuser, the air stream entering the combustion chamber will be presumed at some moderate or low supersonic Mach number with a static pressure more than one tenth of the sea

level atmosphere and with a static temperature not in excess of  $1000^{\circ}\text{K}$ . We wish to explore the various technical aspects of burning hydrogen in such a supersonic air stream to generate high temperature gas mixture of the combustion products of  $\text{H}_2$ ,  $\text{O}_2$  and  $\text{N}_2$  for expansion through a nozzle.

The injector that supplies  $\text{H}_2$  gas to the air stream can serve as a flame holder provided that the injector base is small. The low speed gas in the recirculating region over the base will be at such a high temperature that the  $\text{H}_2\text{-O}_2$  reactions can not go to completion. This high temperature wake region over the small blunt base will, however, extend only a couple of base diameters downstream. The outer supersonic stream will close the recirculating wake and accelerate the wake mixture back to supersonic speeds further downstream where, the chemical energy locked in the dissociated species may be released upon their recombination at lower temperature. We hope that such recombinations can be accomplished within the space (volume) of the combustion chamber.

With the air stream entering the combustion chamber at low supersonic Mach numbers, a bluff body (as an injector flame holder combination) will have a detached bowshock wave ahead of it, leaving a subsonic flow over and around the entire bluff body. If the diameter of the blunt body is sufficiently small compared with the diameter of the duct of air inflow, the external supersonic stream will eventually close the subsonic flow region behind and around the body. On the other hand, if there should be rows of such small bluff body flame holders arranged and supported like a fine wire mesh across the section, the many bow shocks will merge; and transition to subsonic flows across the entire channel of the inlet will result. There will not be a row of streaks of subsonic wakes to be closed by the surrounding supersonic air flow with ensuing supersonic combustion. To avoid the bow shock we can install a sharp, properly contoured

shroud over a small bluff body. Such may be possible for a handful of flameholders widely separated across the flow channel but not likely over a gigantic array of them held together with supporting structures.

We can avoid the use of structurally supported flame holders altogether by injecting liquid hydrogen transversely as droplets into the supersonic airstream. Each droplet will serve as its own flameholder, while being accelerated downstream by the supersonic flow. A fine spray or a cloud of such droplets, however, can also trigger shock transition of the airstream wrapped around the cloud with subsonic combustion taking place within it. To avoid such bow shocks liquid hydrogen can be injected into the supersonic air stream in the streamwise direction and at comparable velocities such that the supersonic air stream is actually subsonic relative to the droplets. Such droplets, however, play little role of anchoring the flame to the combustor; and the situation is little different from injecting gaseous  $H_2$  to mix with air as two parallel streams of comparable velocities. To hold the combustor length reasonable, we prefer to use some form of injector flame holders, although as few as necessary, to anchor the supersonic combustion downstream. The focus of research on supersonic combustor then becomes the search of means to increase mixing and burning rate of  $H_2$  as a gaseous stream nearly parallel to a supersonic air flow.

The much studied classic flame over a Bunsen burner in a stagnant ambient atmosphere is a flame of parallel stream<sup>(4)</sup>, stabilized by the rim of the burner supplying the fuel. The rim holds the flowing fuel to mix with the ambient air (perhaps with a tiny recirculation region also) so as to initiate the combustion shortly downstream of the rim edge. In so far as downstream combustion is concerned, the flame over a Bunsen burner represents a combustion zone between nearly parallel streams of fuel and air. We often speak of the "flame" with a

"flame front" propagating into the ambient air. The speed of propagation of such a flame normal to the flame front is referred to as the "flame velocity". The flame lasts a few diameters of the burner till all fuels are supposedly burned. This flame length increases with fuel flow velocity. At some large fuel velocity, the flow becomes turbulent and the flame much shorter and more intense. With further increase of fuel velocity, this turbulent flame also lengthens and eventually lifts off from the burner rim, becomes unstable and "flame out". If the ambient air should move downstream with an increasing velocity, similar events will occur but not necessarily in the same sequence, nor with the same details. (This is because of the nonlinearity inherent in the mixing and the combustion dynamics.) The supersonic combustion downstream of a flame holder is a case of the latter where the air velocity is supersonic. Our interest is to establish and hold a steady flame that consumes the fuel within some reasonable flame length. We are therefore apprehensive of the eventuality of excessive stretch out of the flame and flame out at high air speeds. We would like to have the short, intense turbulent flame confined within the combustor.

It is clearly important to understand the dynamics of such a slow deflagration flame, propagating into a premixed fuel-air reservoir. The thermal theory<sup>(4)</sup> offers a rational explanation of the finite small flame velocity in a premixed gas. The hot burned gas behind the flame sends heat through different modes of heat transfer (conduction and radiation) to heat up the unburned premixed gases and ignite them when the mixture reaches some ignition temperature (or some other energy criterion). A steady flame velocity propagating into the unburned mixture can be reached when a unique temperature profile is established across the flame front such that a steady heat flux will bring a stream of unburned gas to the ignition temperature at a constant rate. For the flow of an

idealized homogeneous unburned mixture with radiative heating neglected in one space dimension, we have been able to determine the characteristic temperature profile and estimate quite reasonably the flame velocity from material properties. For a heterogeneous mixture, there is of course the additional question of mass transport to bring the fuel and the air together to establish a suitable mixture with some reasonable ignition temperature and heat of combustion. When the appropriate range of equivalence ratio is established, the thermal theory may apply locally. Then the computational solution of such an aerotherodynamic problem of heterogeneous combustion can be carried out with detailed treatments of mass, momentum and energy transports. The flame will have a unique profile and a finite small thickness commensurate with the small diffusivities.

For a premixed  $H_2-O_2$  gas mixture with an adequate equivalence ratio, the reaction time of  $\sim 10^{-6}$  sec, is so small that it may be considered as instantaneous. Thus, in a heterogeneous mixture of  $H_2$  and  $O_2$  gas, combustion products and heat of reaction may be considered as released instantly whenever an adequate (usually stoichiometric) equivalence ratio is reached. The combustion products and heat diffuse into the unburned gas mixture while being convected or carried downstream by the mixture motion. The thermal aspects may be neglected. The reaction front thus becomes determined entirely by the inter-diffusion of the reactants and the combustion products. This flame is known as the "diffusion flame"<sup>(4)</sup>. The flame velocity can be simply illustrated within the one dimensional framework just as in the thermal theory. In view of the comparable magnitudes of the thermal and the mass diffusivities, it is not surprising that the flame velocities estimated with the thermal and the diffusion theories are comparable; and both can be made to compare favorably with the



various experimental findings. The experimental measurements of flame velocity are also quite varied. They can be based on volumetric or mass fluxes measurements of the combustion products or of the influx of the unburned mixture. Moreover, the flame front is generally curved. The determination of the flame velocity normal to the front needs an estimate of the curvature of such fronts. The curved fronts may be "determined" in different apparatus based upon observations of different parameters such as the global temperature or the concentrations of different reactive intermediate species etc. Such measured values of  $H_2-O_2$  flame velocity vary appreciably; but are generally in agreement, of the order of m/sec. under atmospheric pressure and for unburned mixtures at room temperatures. Both pressure and temperature cause some variations of the flame velocity but within the order of magnitudes. In view of all these uncertainties some hesitate to choose specific reaction models for heterogeneous systems, and adopt some global mixing rate(s) on the fuel-air boundary so that the global conservation relations can determine the progress of the reactive flow system. They are also as successful in reproducing experimental results when the mixing rates are chosen properly.

When the flow becomes turbulent, the effective diffusivities and the mixing rates increase from their laminar values with corresponding increase of the burning rate as measured experimentally. The effect of turbulence is accommodated by empirical changes of the diffusivities or the mixing rates, without any concern of the details of turbulence dynamics. A classical attempt to rationalize the role of turbulence on flame velocity is based on the observation that turbulent velocity fluctuations tend to disrupt and alter the direction of propagation of the laminar flame. The turbulent flame in a premixed unburned gas can thus be looked upon as a "Wrinkled Laminar flame" with the

increase of mass-burning rate accounted for by the area increase of the wrinkled flame<sup>(4)</sup>. The "wrinkling" is a purely kinematic effect, much more effective for small scale disturbances. Since momentum transport is supposed to be most effectively carried out by small scale eddies, the concept of wrinkled flame would suggest that the effective turbulent flame velocity (or burning rate) can be scaled up from the laminar flame velocity as the turbulent eddy diffusivity for momentum transport may be scaled from the laminar kinematic viscosity.

The supersonic air flow entering the combustor inlet at the operating altitudes of a SCRAMJET is presumably laminar because of the low density of the entering atmosphere. With the laminar flame velocity of the order of a few m/sec., the flame front propagating into a supersonic stream will be inclined to the stream direction at an angle of  $< 1^\circ$ , i.e. the length of the combustion region in a supersonic combustor would be  $10^2$  or more times the spacing of the flame holders across the section. We are anxious to increase the flame velocity (or the mixing rate) so as to avoid the excessively long combustor, since we do not want to use too many flame holders. When the flow becomes turbulent, the momentum exchange coefficient increases by  $10^2$  to  $10^3$  folds. If the concept of wrinkled flame should be any guide, we could secure similar increase of the burning rate with turbulent combustion; and we would have complete combustion within some reasonable length of a supersonic combustor. Therefore, as early as 1960's, various windtunnel experiments were performed to burn hydrogen in parallel supersonic air flows, such as jet mixing, flows over wake or rearward facing steps with natural and stimulated turbulence. It was hoped to find effective means of stimulating turbulent mixing so as to achieve fast burning. Early experimental results<sup>(5)</sup> show that the rate of spread of combustion into the supersonic air stream is somewhat improved but far from what is expected or

desired. Such results appear consistent with the findings at low speeds that the turbulent flame velocities obtained in laboratories are generally 2 or 3 times the laminar values, not increased by an order of magnitude<sup>(4)</sup>. Since turbulent diffusivities of mass, momentum and energy are generally believed to be of the same order of magnitudes, the thermal and/or the diffusion flame theory would offer the same outlook as the wrinkled flame theory. We know that natural and stimulated transition lead to different turbulent flows. Different transitional and turbulent flows can have different mixing rates. There is therefore always the possibility that some mode(s) of stimulating transitional and turbulent flows may lead to comparable mixing rates of mass, momentum, energy and hence the burning rate or the flame velocity. The search of such a mode of controlling and/or stimulating transition of a supersonic flow has been much intensified in the interest of SCRAMJET since 1970's.

More extensive windtunnel tests better simulating the SCRAMJET operating conditions have been performed along with analyses and computations<sup>(6)</sup>. The objective is to increase the mixing and/or the burning rate in a supersonic air stream by stimulating fast transition and intensifying flow turbulence. It helps to study the dynamics of transition. Hence the instability of small disturbances in parallel flows has been extensively studied experimentally and computationally. The rapid development of computational fluid dynamics (and hence aerothermodynamics) and the increasing availability of supercomputers have greatly increased the expectations of an eventual, if not prompt, helpful understanding of transitional flow dynamics. Current attention<sup>(7)</sup> appears to be limited to the evolution of an isolated unstable disturbance in a parallel flow. The instability of small disturbances is widely conceived as a prerequisite of natural transition to turbulence in a well-controlled flow system. The study of

the growth of unstable disturbances and their eventual course of evolution can surely shed light on the dynamics of the early phase(s) of flow transition although such natural transition is too slow for our purposes. The dynamics how a sufficiently large disturbance will bring about instantaneous transition can be quite different. We need much deeper understanding of the transition dynamics which involves, at some later stages of evolution, a rich assortment of complex structural and topological flow configurations in three space dimensions as have been observed experimentally<sup>(8)</sup>. We should understand better the structure and the dynamics of transitional flows in the late stages. Moreover, with fast transition, supersonic combustion will be accomplished largely in the fully turbulent state. An adequate understanding of how turbulence influences the various transport phenomena, and how they increase the burning rate can be more than helpful.

Current research efforts on fully turbulent flows rely heavily on the coordinated diagnostic experiments and computational simulations to establish (or validate) some suitable "turbulence Modeling" for some specific range of applications. Numerous models, algebraic or differential, have been constructed, tested and claimed to be successful for specific applications<sup>(8)</sup>. To validate or to establish a model as better than the classical eddy diffusivities or mixing coefficients has, however, not been a straight forward task even for non-reactive flows. Such a validated model still has to be extended to include the effects of physico-chemistry and further validated for application to the reactive  $H_2-O_2$  system of supersonic combustion in a SCRAMJET. It is difficult to see how such an approach can help to achieve higher mixing or burning rate for the supersonic combustor. We have to develop better understanding of transitional and turbulent shear flows to make meaningful progress. In the next section, we shall review

the current status of our understanding of transition and turbulence and examine the various implications.

#### 4. Transition, Turbulence and Combustion

Turbulence is generally recognized as a diffusive phenomenon with diffusivities (exchange or transport coefficients) much larger than those of laminar flows under molecular chaos. It has proven its usefulness in correlating turbulent data in engineering applications. The turbulent eddy diffusivities are not material properties like laminar diffusivities but heavily dependent on the dynamic situations and flow configurations. Transition from laminar to turbulent flow states is often idealized as occurring instantly at some "critical Reynolds number", some "reliable estimate" of which is often considered crucial in specific engineering applications. In reality, natural transition extends over a sizable region covering a decade of  $Re$  around the critical value. The physical length of this transition region is many times the length of the upstream laminar flow over an equivalent flat plate. The concept of critical transition Reynolds number is merely to facilitate analysis and understanding when the length scale of our interest is meaningfully larger than that of the transition region. To bring about quick transition over a small region and around some smaller critical Reynolds numbers, we have to consider the dynamics of transitional flows.

Transitional flow is not an extension of the "fully" turbulent flow (or any other unique entity) at reduced intensities. It is structurally very complex, involving sporadic, abrupt, propagating large disturbances, each surrounded by a local region of chaotic flow or turbulence<sup>(8)</sup>. It may expand in its own contorted ways accompanied by the decay of the peak disturbances. These are relatively "large" scale (length and time) phenomena and often "coherent" when averaged over a specific flow configuration as "ensemble averages". Such sporadic disturbances occur with increasing frequency during transition toward

turbulence while the surrounding local "turbulent" regions overlap and agglomerate. There is no unique "profile". Such large disturbances may have been introduced by external events, including the incursion of neighboring turbulent flows (external turbulent free stream). In an isolated fields such as a parallel laminar shear flow small disturbances can become unstable at sufficiently large Reynolds numbers and grow to large amplitudes. Such flow instabilities of small disturbances have been observed to generate structurally complex flows in three space dimensions before reaching large amplitudes. Such complex flow can evolve and amplify further and generate local turbulent regions around them. The sporadic nature of the unstable and of the external large disturbances small disturbances leads to the sporadic occurrence of local turbulent regions.

At any spatial position, in a transitional flow field, the flow intermittently "laminar" and "turbulent" as this point is uncovered or covered by the sporadic local turbulent region(s)<sup>(8)(9)</sup>. We call the averaged fractional time, during which the flow at a given point is turbulent, the "Intermittency Factor". It is near zero at the beginning of transition and near unity as the fully turbulent condition is approached. This intermittency factor does vary monotonically throughout the transition region from 0 to 1, much like the average temperature across a flame front. The turbulent intensity, however, varies erratically throughout a transition region. When we take some average of some turbulent quantities, like mixing rates, over a sufficiently long period of time over many laminar and turbulent periods, the intermittency factor tends to be more heavily weighted for higher order nonlinear quantities. This introduces serious complications in interpreting and understanding the mixing rates and the burning rates in such transitional flows<sup>(10)</sup>. We may be able to avoid such the

transition to turbulence in a very short time and over a very small spatial region such that the combustor is almost entirely filled with fully turbulent supersonic combustion. How to achieve such fast and local transition to turbulence is a subject of intense research and development. It has to depend at present heavily on experimentation with minimal theoretical guidance.

Current emphasis of this transition research is the instability and the evolution of unstable small disturbances in a parallel laminar flow. This is the earliest stage of the transition processes. Most stability analyses and computations treat sufficiently small planar or axisymmetric disturbances that permit linearized superposition. The determination of the stability boundary for a given type of such small disturbances involves the solution of complicated eigen value problems that are nonlinear. The stability boundary is therefore very sensitive to the flow field configurations and the type of disturbances. When such unstable 2D disturbances grow to modest amplitudes, they become three dimensional when their amplitudes are still modest. They generate disturbances of different types and frequencies which have to be analyzed as nonlinear phenomena, at least through quasi-linearization in the form of successive higher order instabilities. Some computational solutions of secondary instability have succeeded to provide vivid simulation of the rolling up of an amplifying planar disturbance observed in experiments<sup>(7)</sup>. Although still quite a way off from the large physical disturbances capable of triggering local solution bifurcation into turbulent states, such computations are certainly steps in the right direction to gain insight of the dynamics of sudden transition into local turbulence. Computational solutions of the full Navier Stokes system have also have carried out to simulate the events how an isolated large disturbance will or will not bring about the emergence of a local turbulent region<sup>(9)</sup> and how the various



local turbulent regions around different large disturbances will agglomerate and interact<sup>(11)</sup> in the approach to some fully turbulent state. Such solutions are interesting but failed to suggest how the desired large disturbance may be generated in practical flow system to produce instant transition locally. We hope, nevertheless, that some useful results could be forthcoming from such studies of the late stages of development. In any cases, a good understanding of the fully turbulent shear flow is necessary since we wish to have supersonic combustion in such turbulent flows.

The classical treatment of the fully turbulent shear flows has been limited to the statistical averages or mean flow properties of practical interest. Thus, the Reynolds transport equations for the turbulent mean shear flow fields of an incompressible fluid were given a century ago with the second higher order correlations of turbulent velocity fluctuations known as the Reynolds stresses. Turbulent models as constitutive relations to express such higher order correlations in terms of the mean flow properties are needed to solve them. By presuming analogy between turbulent and molecular chaos, the gradient type diffusion models have been introduced and widely accepted. Such algebraic models in terms of diffusivities, mixing lengths etc. have served much useful purposes in correlating experimental data; and have provided the framework of our earlier discussions. Since around 1930's the statistical theory of turbulence has been extensively developed for Isotropic Homogeneous Turbulence in both the physical and the spectral space. For the determination of its energy spectral function, closure hypothesis to relate the unknown higher orders is also needed correlations to those of lower orders just as the modeling of those turbulent transport properties in turbulent shear flows. Thus shear flow turbulence modeling is taken as the analog of closure in IHT. Encouraged by the many ad hoc

closure schemes of IHT, numerous ad hoc procedures have been developed for shear flow turbulence modeling with much more empiricism and many dubious interpretations of "Statistical inferences from IHT. Even if some such complicated shear turbulence models should prove to be superior and "validated", we still cannot identify, the turbulence dynamics among the many hypotheses and empiricism, for extension to compressible fluid flows and with combustion reactions. Much more difficult and more complex phases of model development, of their computation solutions and their validations, still lie ahead if its is to be helpful to the SCRAMJET development.

The deterministic theory <sup>(9)(10)</sup> based on some abstract mathematical development in modern nonlinear dynamics presents a much different outlook. The evolution of an unstable disturbance in a nonlinear field leads to rapid bifurcation into a new solution state, likely of higher dynamic dimensions. Such a bifurcation process is fast and complex and much varied. The new bifurcated state can become unstable locally and proceed toward another bifurcation. Such successive solution bifurcations, when the parameter of the nonlinear system lie in a suitable range, leads to chaotic solutions or chaos i.e the "mathematical turbulence". If we firmly believe that the Navier-Stokes system represents the transient dynamics of the flow systems, the successively bifurcating solution of an initial-boundary value problem of the Navier-Stokes system should represent fluid turbulence. Its course of evolution of a given initial disturbance is completely determined. The "turbulence dynamics" is a property of the nonlinear Navier-Stokes system alone. There is no need of "Closure Hypothesis" nor turbulence modeling." Chaotic solutions differ with different initial data (and flow configurations). If the initial (and/or boundary ) data are uncertain, the resulting turbulent field would subject to the statistics of the uncertain data

in addition to the statistics of the chaos of the N.S. dynamics. If the initial data are fully presented, the N.S. dynamics determines the chaos or turbulence to follow. Thus modern Nonlinear Dynamics suggests encourages the search of means for fast transition within the N.S. dynamics; but the futility of turbulence modeling to alter the N.S. dynamics without paying attention to the role of initial data.

The solution referred to above is the genuine solution of the N.S. system treated in the abstract mathematics. Any useful computed approximation of such nonlinear evolution problems must follow the appropriate branch of the bifurcated states of the genuine solutions and hence cannot tolerate any numerical artifices due to inherent chaos or deliberate smoothing. Such computed approximations must of course be validated against experimental observations. Therefore we computed the evolution of an individual impulsive disturbance in a uniform shear flow at  $Re \sim 3000-300$  of some velocity or vorticity components of magnitudes  $10^{-2}$  to 10. Scores of such computed results have been found to fall into three classes as have been observed in physical experiments.

(i) Small disturbances quickly die out, restoring the undisturbed uniform shear flow within the computational accuracy.

(ii) Disturbances of intermediate strengths "explode" into a turbulent field that decay as rapidly to restore some distorted laminar flow.

(iii) A sufficiently large disturbance generates a high intensity oscillatory core with a large local turbulent region propagating slowly into the surrounding laminar region. The core develops into a pair of counter rotating vortices in the streamwise direction preceded by a local jet stream away from the plate and followed by a collapsing column of fluid toward the plate. The

whole pattern drifts in the main stream direction as a coherent entity. The structure appears to be driven by the associated pressure disturbances with multi-peaks and valleys, with peak magnitudes governing if a local turbulent region will develop. Similar computations for free turbulence is in progress, while those for compressible fluids with or without chemical reactions are being planned.

The deterministic theory encourages the search of initial-boundary disturbances that will give fast transition. Since ignition is an unstable process accompanied by a large energy release it can generate turbulence rapidly. Theoretically speaking, the nonlinear mass and energy sources in the nonlinear system of aerothermodynamics, are capable of generating chaos through repeated bifurcation by themselves, besides altering the bifurcating sequences of a nonreactive system. We note that turbulence intensity has been measured across a "laminar flame" to rise from the residual value in the unburned "laminar" gas stream to significantly larger values in the downstream burned gas<sup>(11)</sup>. The so called "laminar flame velocity" may have been benefited by this self generated turbulence. If so, the fully "Turbulent flame velocity" may not be expected to increase by order(s) of magnitude over such "laminar" flame velocity".

The old experiment of turbulence measurements across a laminar flame should be repeated with more modern techniques of turbulence measurements, and not likely limited to the "turbulence intensity" alone. Enhancing flow turbulence will remain a valid concept for improving supersonic combustion although its potential might not be as big as hoped for.

With ignition enhanced mixing, a fuel rich ( $H_2-O_2$ ), slightly under expanded rockets may serve as a good injector flame holder in a supersonic combustor because the rocket exhaust is highly turbulent and with numerous ignition

sources. Such an arrangement has been experimented within "ram rockets" in 1950's. A simple one-dimensional analysis of such a ram rocket configuration as a propulsive device was carried out. The one dimensional flow implies instant mixing. The rate of heat addition or burning rate was estimated from the turbulent flame speed propagating into the unburned mixture. With the small turbulent flame velocity compared with the supersonic inlet air flow, the combustion of such "premixed" gases would take place over  $\sim 10^2$  times the rocket spacing as mentioned in Section 3. It is important to recognize that even if the combustion should proceed as a detonation wave, the combustion front would still be inclined to the mean flow direction at an angle of  $\sim 1/M$  comparable to the oblique shock angle. The speed of a deflagration front is an order of magnitude smaller and the combustion region correspondingly larger. It appears therefore, that SCRAMJET will necessarily need a long combustion region with a substantial fraction of heat release, in the thrust nozzle downstream. The engine performance would be somewhat compromised, but can remain adequate for many missions such as the Mach 6 cruiser. The elementary one dimensional analysis of the ram-rocket suggests the upper limit of its thrust to be comparable to although less than the sum of what could be derived from the rockets and the subsonic ramjet separately.

## 5. Beyond SCRAMJET

The segment of airbreathing corridor (Fig.. 2) in which SCRAMJET will operate is bounded from below at Mach numbers  $\sim 3$  and altitudes  $\sim 30$  Km by the need of Ram pressure recovery. The low altitude boundary at increasing Mach numbers is imposed by the tolerable aerodynamic heat flux or the heat shield.

The upper boundary represents a combustion limit. At higher Mach numbers it is, essentially a horizontal line at about  $\sim 60$  Km., where the ambient air density is judged too low to give a combustible mixture, i.e. an inflammability limit. The corridor thus extends at constant altitude to higher flight Mach numbers by tolerating the rapidly rising drag and heat flux. SCRAMJET appears to be an ideal hypersonic propulsion unit for missions like Mach 6 cruiser at  $\sim 40$  Km altitude with some room for maneuver. To cruise at a significantly higher altitude is not possible and to cruise at larger Mach numbers pays high penalty. It cannot provide its payload with enough kinetic energy to coast into a Mach 25 or 30 low orbit. An aero-assisted orbital transfer vehicle (ADTV), with SCRAMJET has to be boosted back into its new orbit with additional rocket power. There is therefore little incentive to take the severe penalties in lowering an orbital vehicle to such a low altitude and low Mach number for SCRAMJET maneuver before being boosted into its new orbit.

To increase the kinetic energy of the payload, the power plant must generate net thrust  $T-D$ . The vehicle drag  $D$  is linearly proportional to air density, largely independently of the combustion processes. The thrust  $T$  of the engine is proportional to the rate of energy release from the combustion processes. For binary gaseous combustion reactions like  $H_2$  and air, this energy release rate is proportional to the square of the gas density,  $\sim \rho^2 C_H C_O \exp [-A/(RT)]$  if the second order combustion processes might be "frozen" at the idealized design condition. If a power plant possesses a given thrust margin  $T_0-D_0$  at some reference state, say 30 Km and Mach 4; for the scramjet, the engine thrust  $T$  will drop much faster than the drag  $D$  as air density  $\rho/\rho_0$  drops rapidly with increasing altitudes. A large thrust margin  $T-D$  will disappear within a couple of atmospheric scale height. (Fig. 5a). The thrust margin will actually vanish

much sooner with the deteriorating combustor performance at off-design conditions, and especially as the chamber pressure (density) falls toward the inflammability limit. With second order gas phase combustion reactions, poor high altitude engine performance is inevitable.

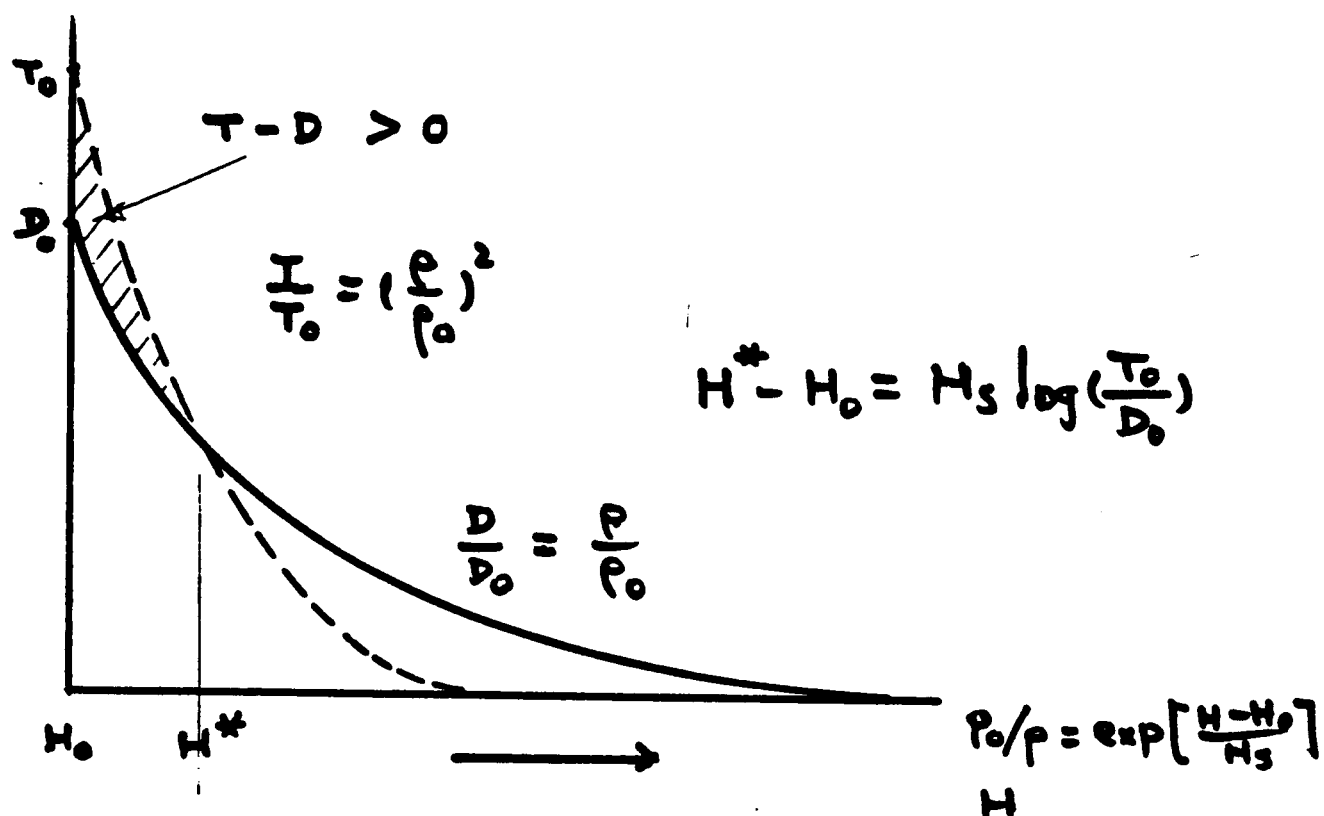
If combustion could be implemented through first order reaction(s) the situation will improve significantly. A first order combustion reaction would imply linear fall off of engine thrust with density. Thus, as indicated in Fig. 5b, a positive thrust margin at the design point would remain positive through all altitudes although the magnitude of the thrust margin T-D would decrease linearly with density. A catalytic surface reaction of  $O_2$  onto a molecular layer of hydrogen adsorbed on the surface of some noble metal like platinum will provide such a first order reaction. This is because the hydrogen concentration on the surface is determined by the surface potential of the metal with sufficient supply of  $H_2$  gas. Air as a mixture of  $N_2$  and  $O_2$  incident onto the surface will mostly be intercepted by the tightly packed layer of adsorbed  $H_2$  molecules. Very few of the incident molecules will penetrate into the metallic surface. Molecular encounters of the energetic incident  $O_2$  and the absorbed  $H_2$  molecules will lead to oxidation reactions.

An outstanding issue in considering air breathing propulsion systems (and hypersonic vehicles) at such high altitudes is that the aerodynamic environment must not be considered from the continuum fluid but rather the rarefied gas point of view. The reaction products will leave the surface as may be dictated by the conservation laws. They could intercept and deflect the incident  $O_2$  molecules away from the surface; but such collisions are of second order and fall off as the square of density, negligible at higher altitudes to keep the catalytic surface reaction of first order.

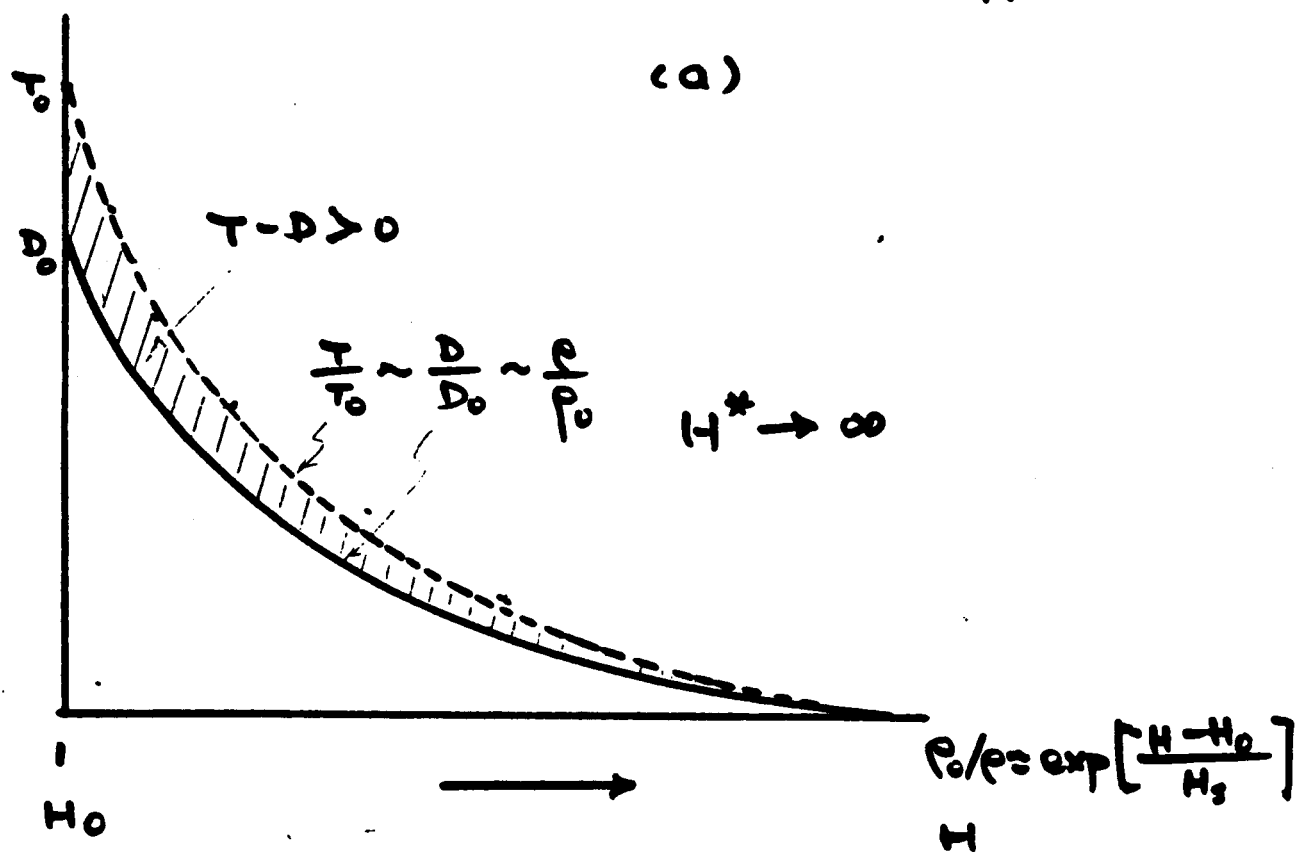
An outstanding issue in considering air breathing propulsion systems (and hypersonic vehicles) at such high altitudes is that the aerodynamic environment must not be considered from the continuum fluid but rather the rarefied gas part of view. The rarefied gas dynamics in the form of Kinetic Theory of gases and its extensions is over a century old; but mostly for near-equilibrium distributions. Direct Simulation Monte Carlo method (DSMC) of computational solution of rarefied gas dynamics problems has become highly popular. Its application to hypersonic rarefied gas flows with  $MK_N \gg 1$ , is fundamentally not quite consistent, however. It contains, moreover, much empiricism to facilitate the reproduction of preconceived results but prevent understanding of physical dynamics needed for the design of hypersonic vehicles. Alternative methods for treating the mean flow properties are being developed and tested (13)(14). Some are similar to the Navier-Stokes system for a nonequilibrium gas mixture with scattering interaction. Much remains to be done both as to the form of the fundamental equations and the subsidiary relations of scattering interactions off and on the surface. On surfaces of catalytic combustion the interaction will be chemically reactive.

A hypersonic propulsive system based on catalytic surface combustion promises to deliver net thrust all the way to orbital altitudes. The absolute magnitudes of the net thrust decreases linearly with air density but remains comparable to and larger than the prevailing drag. Since the thrust delivered by





(a)



(b)

the device is small and controllable at near orbital altitudes, it can replace the small rocket motor for injecting the vehicle into its desired orbit precisely. It can keep a satellite in station or change its orbit. Such an engine can deliver a much larger total impulse or velocity change if it is allowed enough time to scoop up as much needed air along its trajectory. Thus, an AOTV maneuver can be accomplished at altitudes much above 40 ~ 50 Km, although it may need a few orbits.

Catalytic surface reaction of  $H_2$  with incident air at lower speeds and higher densities are at least as likely as at higher altitudes. Such a propulsive device will therefore remain operable at 30 ~ 50 Km altitudes to compete with scramjet, and possibly to overlap with the operating range of subsonic combustion ramjet with variable geometry (Fig. 2,3). The supersonic combustion ramjet (SCAMJET) is under intensive research and development and likely to succeed in fulfilling its specific objective. The catalytic surface combustion Ramjet may be a valuable addition and useful extension of the supersonic combustion ramjet as a more versatile hypersonic propulsion system. It poses new frontiers of research and development in combustion, aerodynamics and propulsion systems, quite different from those presented by SCRAMJET.

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# Report Documentation Page

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16. Abstract. This program is to develop an analytic method for reducing SUMS data for the determination of the undisturbed atmosphere conditions ahead of the shuttle along its descending trajectory. It is divided into an internal flow problem, an external flow problem and their matching conditions. Since the existing method of Direct Simulation Monte Carlo (DSMC) failed completely for the internal flow problem, the emphasis is on the internal flow of a highly non-equilibrium, rarefied air through a short tube of a diameter much less than the gaseous mean free path. A two fluid model analysis of this internal flow problem has been developed and studied with typical results illustrated. A computer program for such an analysis and a technical paper published in Lecture Notes in Physics No. 323 (1989) are included as Appendices 3 and 4. A proposal for insitu determination of the surface accommodation coefficients $\sigma_t$ and $\sigma_e$ is included in Appendix 5 because of their importance in quantitative data reduction. A two fluid formulation for the external flow problem is included as Appendix 6 and a review article for AIAA on Hypersonic propulsion, much dependent on ambient atmospheric density, is also included as Appendix 7.					
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